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FILE COVERS 1907 - 15 Jul 2004  VOL 141 ISS 3
FILE LAST UPDATED: 14 Jul 2004  (20040714/ED)

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'OBI' IS DEFAULT SEARCH FIELD FOR 'HCAPLUS' FILE

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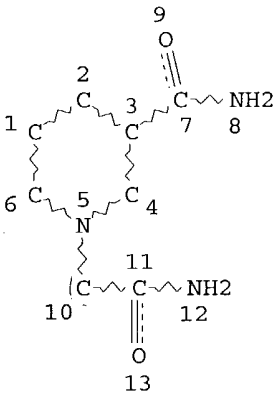


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GRAPH ATTRIBUTES:
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STEREO ATTRIBUTES: NONE
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L28  ANSWER 1 OF 11  HCAPLUS  COPYRIGHT 2004 ACS on STN
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AN 2002:835107 HCAPLUS
DN 139:414
ED Entered STN: 04 Nov 2002
TI Improved cancer treatment with enzyme technology
CS Enact Pharma, Enact Pharma plc, Salisbury, SP4 0JQ, UK
SO sp2 (2002), 1(8), 22, 24-25
CODEN: SPSUCF; ISSN: 1476-184X
PB Avakado Ltd.
DT Journal
LA English
CC 1-6 (Pharmacology)
AB The treatment of solid cancers with drugs often has limited effectiveness because, in general, the drugs do not specifically target the cancer. Many strategies have been devised to improve tumor selectivity, but researchers at the biopharmaceutical company Enact Pharma plc believe that the catalytic properties of tumor-associated enzymes may be used to provide effective cancer therapy using simple, low-mol.-weight compds. One approach to cancer therapy being pursued by Enact takes advantage of the fact that some enzymes are over-expressed in cancer cells and can be used to selectively convert a prodrug into a potent anticancer agent. Ideally, the prodrug should be an inert, low-mol.-weight mol. that can be chemical modified by the enzyme (e.g., by reduction or scission) to generate a pharmacol. active mol. Local generation of the active species should ensure that toxicity to normal human tissues is kept to a min. Researchers at Enact have discovered a unique biochem. activity in a human enzyme called NQO2 (NAD(P)H quinone oxidoreductase 2). This enzyme is normally inactive, even in the presence of known biogenic enzyme co-substrates such as NAD(P)H. Enact has switched on the enzyme NQO2 and demonstrated that it is an aerobic nitroreductase. This was achieved by administration of a simple dihydropyridine derivative, designated as EP-0152R (1-carbamoylmethyl-3-carbamoyl-1,4-dihydropyridine). Enact has exploited the discovery by using the switched on NQO2 to convert a prodrug called CB 1954 [5-(aziridin-1-yl)-2,4-dinitrobenzamide] into a potent cytotoxic agent. The bioactivation of CB 1954 allows its cytotoxicity to be dramatically increased, with differences of up to 10,000-fold observed against some human tumor cell lines. In fact, CB 1954 acts as a difunctional alkylating agent once it has been activated by the enzyme NQO2. In the presence of EP-0152R, NQO2 was found to catalyze the aerobic reduction of CB 1954 to the hydroxylamino derivative, 5-(aziridin-1-yl)-4-hydroxylamino-2-nitrobenzamide. This compound is highly toxic to cells, even to those resistant to CB 1954, and can form inter-strand cross-links in their DNA. As human cells cannot normally activate CB 1954 and NQO2 is over-expressed in a number of tumor types, Enact believes that this system has considerable potential as a targeted anti-tumor therapy. Preclin. studies have shown that a combination of EP-0152R and CB 1954 is effectively cytotoxic toward a number of human tumor cell lines. Colorectal, prostate and liver cancer cell lines were particularly sensitive, but breast cancer cells were found to contain little NQO2, so were unaffected by the drug combination. The treatment was found to be effective in human prostate and colorectal tumor xenograft models, causing significant regressions and delays in tumor growth, with little toxicity.
ST antitumor prodrug CB 1954 activation NADPH quinone oxidoreductase 2; cancer therapy prodrug activation tumor specific enzyme
IT Intestine, neoplasm
(colorectal; improved cancer treatment with enzyme technol. involving prodrug (CB 1954) activation by tumor-specific enzyme (NAD(P)H-quinone oxidoreductase 2))
IT Antitumor agents
Human
Liver, neoplasm

Prostate gland, neoplasm
(improved cancer treatment with enzyme technol. involving prodrug (CB 1954) activation by tumor-specific enzyme (NAD(P)H-quinone oxidoreductase 2))

IT Drug delivery systems
(prodrugs; improved cancer treatment with enzyme technol. involving prodrug (CB 1954) activation by tumor-specific enzyme (NAD(P)H-quinone oxidoreductase 2))

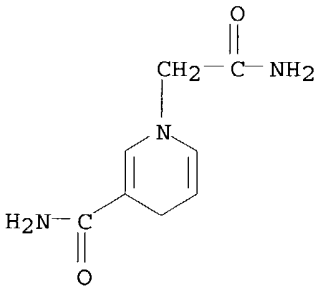
IT **64881-21-6**, EP 0152R
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); PKT (Pharmacokinetics); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(enzyme activator; improved cancer treatment with enzyme technol. involving prodrug (CB 1954) activation by tumor-specific enzyme (NAD(P)H-quinone oxidoreductase 2))

IT 667919-86-0
RL: BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(improved cancer treatment with enzyme technol. involving prodrug (CB 1954) activation by tumor-specific enzyme (NAD(P)H-quinone oxidoreductase 2))

IT 21919-05-1, CB 1954
RL: ADV (Adverse effect, including toxicity); DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(prodrug; improved cancer treatment with enzyme technol. involving prodrug (CB 1954) activation by tumor-specific enzyme (NAD(P)H-quinone oxidoreductase 2))

IT **64881-21-6**, EP 0152R
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); PKT (Pharmacokinetics); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(enzyme activator; improved cancer treatment with enzyme technol. involving prodrug (CB 1954) activation by tumor-specific enzyme (NAD(P)H-quinone oxidoreductase 2))

RN 64881-21-6 HCAPLUS
CN 1(4H)-Pyridineacetamide, 3-(aminocarbonyl)- (9CI) (CA INDEX NAME)



L28 ANSWER 2 OF 11 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2000:597759 HCAPLUS
DN 133:275962
ED Entered STN: 29 Aug 2000
TI Bioactivation of 5-(aziridin-1-yl)-2,4-dinitrobenzamide (CB 1954) by human NAD(P)H quinone oxidoreductase 2: a novel co-substrate-mediated antitumor prodrug therapy

AU Knox, Richard J.; Jenkins, Terence C.; Hobbs, Stephen M.; Chen, Shiuan; Melton, Roger G.; Burke, Philip J.
CS Enact Pharma Plc, Salisbury, SP4 0JQ, UK
SO Cancer Research (2000), 60(15), 4179-4186
CODEN: CNREA8; ISSN: 0008-5472
PB American Association for Cancer Research
DT Journal
LA English
CC 1-6 (Pharmacology)
Section cross-reference(s): 7
AB A novel prodrug activation system, endogenous in human tumor cells, is described. A latent enzyme-prodrug system is switched on by a simple synthetic, small mol. co-substrate. This ternary system is inactive if any one of the components is absent. CB 1954 [5-(aziridin-1-yl)-2,4-dinitrobenzamide] is an antitumor prodrug that is activated in certain rat tumors via its 4-hydroxylamine derivative to a potent bifunctional alkylating agent. However, human tumor cells are resistant to CB 1954 because they are unable to catalyze this bioactivation efficiently. A human enzyme has been discovered that can activate CB 1954, and it has been shown to be commonly present in human tumor cells. The enzyme is NQO2 [NAD(P)H quinone oxidoreductase 2], but its activity is normally latent, and a nonbiogenic co-substrate such as NRH [nicotinamide riboside (reduced)] is required for enzymic activity. There is a very large (100-3000-fold) increase in CB 1954 cytotoxicity toward either NQO2-transfected rodent or nontransfected human tumor cell lines in the presence of NRH. Other reduced pyridinium compds. can also act as co-substrates for NQO2. Thus, the simplest quaternary salt of nicotinamide, 1-methyl-3-carboxyamidopyridinium iodide, was a co-substrate for NQO2 when reduced to the corresponding 1,4-dihydropyridine derivative Increased chain length and/or alkyl load at the 1-position of the dihydropyridine ring improved specific activity, and compds. more active than NRH were found. However, little activity was seen with either the 1-benzyl or 1-(2-phenylethyl) derivs. A neg. charged substituent at the 3-position of the reduced pyridine ring also negated the ability of these compds. to act as cosubstrates for NQO2. In particular, 1-carbamoylmethyl-3-carbamoyl-1,4-dihydropyridine was shown to be a co-substrate for NQO2 with greater stability than NRH, with the ability to enter cells and potentiate the cytotoxicity of CB 1954. Furthermore, this agent is synthetically accessible and suitable for further pharmaceutical development. NQO2 activity appears to be related to expression of NQO1 (DT-diaphorase), an enzyme that is known to have a favorable distribution toward certain human cancers. NQO2 is a novel target for prodrug therapy and has a unique activation mechanism that relies on a synthetic co-substrate to activate an apparently latent enzyme. Our findings may reopen the use of CB 1954 for the direct therapy of human malignant disease.
ST antitumor prodrug CB1954 activation quinone oxidoreductase
IT Alkylating agents, biological
Antitumor agents
(bioactivation of CB 1954 by human NAD(P)H quinone oxidoreductase 2 and novel co-substrate-mediated antitumor prodrug therapy)
IT Drug delivery systems
(prodrugs; bioactivation of CB 1954 by human NAD(P)H quinone oxidoreductase 2 and novel co-substrate-mediated antitumor prodrug therapy)
IT 21919-05-1, CB 1954
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)
(bioactivation of CB 1954 by human NAD(P)H quinone oxidoreductase 2 and novel co-substrate-mediated antitumor prodrug therapy)

IT 667919-86-0
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(bioactivation of CB 1954 by human NAD(P)H quinone oxidoreductase 2 and novel co-substrate-mediated antitumor prodrug therapy)

IT 952-92-1P 7145-37-1P 17750-23-1P 17750-24-2P 58880-44-7P
64881-21-6P 89080-16-0P 99362-74-0P 114554-11-9P
115503-79-2P 218443-91-5P 300367-67-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(bioactivation of CB 1954 by human NAD(P)H quinone oxidoreductase 2 and novel co-substrate-mediated antitumor prodrug therapy)

IT 1341-23-7D, Nicotinamide riboside, reduced
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(bioactivation of CB 1954 by human NAD(P)H quinone oxidoreductase 2 and novel co-substrate-mediated antitumor prodrug therapy)

IT 98-92-0, Nicotinamide
RL: RCT (Reactant); RACT (Reactant or reagent)
(bioactivation of CB 1954 by human NAD(P)H quinone oxidoreductase 2 and novel co-substrate-mediated antitumor prodrug therapy)

IT 5463-59-2P 6456-44-6P 13076-43-2P 51652-08-5P 52047-79-7P
97009-81-9P 106047-77-2P 109942-74-7P 126298-92-8P
218443-88-0P 218443-90-4P 218443-92-6P 218443-93-7P
300367-54-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(bioactivation of CB 1954 by human NAD(P)H quinone oxidoreductase 2 and novel co-substrate-mediated antitumor prodrug therapy)

RE.CNT 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD

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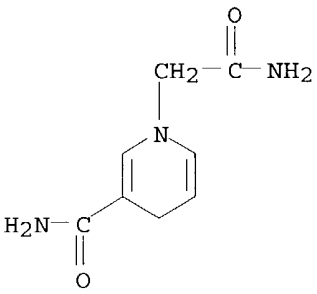
IT **64881-21-6P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(bioactivation of CB 1954 by human NAD(P)H quinone oxidoreductase 2 and novel co-substrate-mediated antitumor prodrug therapy)

RN 64881-21-6 HCAPLUS
CN 1(4H)-Pyridineacetamide, 3-(aminocarbonyl)- (9CI) (CA INDEX NAME)



L28 ANSWER 3 OF 11 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1999:9725 HCAPLUS
DN 130:76160
ED Entered STN: 07 Jan 1999
TI NAD(P)H:quinone reductase 2- and prodrug-based therapeutic systems
IN Burke, Philip John; Knox, Richard John
PA Enzacta R & D Limited, UK
SO PCT Int. Appl., 109 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM A61K047-48
CC 1-6 (Pharmacology)
Section cross-reference(s): 27, 63

FAN.CNT 1

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PI	WO 9857662	A2	19981223	WO 1998-GB1731	19980615
	WO 9857662	A3	19990812		
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	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	GB 2341605	A1	20000322	GB 1999-28237	19980615
	GB 2341605	B2	20020220		

EP 988059 A2 20000329 EP 1998-929555 19980615
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI
GB 2365338 A1 20020220 GB 2001-26082 19980615
GB 2365338 B2 20020403
JP 2002511754 T2 20020416 JP 1999-503953 19980615
HK 1023069 A1 20021011 HK 2000-102240 20000413
HK 1041824 A1 20021115 HK 2002-103701 20000413
US 2003086933 A1 20030508 US 2002-99830 20020313
PRAI GB 1997-12370 A 19970614
GB 1999-28237 A3 19980615
WO 1998-GB1731 W 19980615
US 2000-445865 A1 20000211

AB The invention provides a compound comprising a target cell-specific portion and human NAD(P)H:quinone reductase 2 (NQO2) or a variant or fragment or fusion or derivative thereof which has substantially the same activity as NQO2 towards a given prodrug, or a polynucleotide encoding said NQO2 or said variant or fragment or fusion or derivative Also provided is a recombinant polynucleotide comprising a target cell-specific promoter operably linked to a polynucleotide encoding human NAD(P)H:quinone reductase 2 (NQO2) or a variant or fragment or fusion or derivative thereof which has substantially the same activity as NQO2 towards a given prodrug. The compds. and polynucleotides are useful in a method of treating a patient in conjunction with a suitable prodrug. A method of treating a human patient with a target cell to be destroyed, wherein the target cell expresses NQO2, is provided, the method comprising administering to the patient a prodrug which is converted to a substantially cytotoxic drug by the action of NQO2 and nicotinamide riboside (reduced) (NRH) or an analog thereof which can pass reducing equivalent to NQO2. Preparation and testing of a series of dihydronicotinamide derivative cosubstrates is included.

ST NADH NADPH quinone reductase 2 targeted conjugate therapeutic; polynucleotide NADH NADPH quinone reductase 2 prodrug therapeutic; dihydronicotinamide cosubstrate prepn NADH NADPH quinone reductase 2

IT Fusion proteins (chimeric proteins)
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(NAD(P)H:quinone reductase 2 and cell-targeting moiety; NAD(P)H:quinone reductase 2- and prodrug-based therapeutic systems, and cosubstrate preparation)

IT Antitumor agents
Cytotoxic agents
Drug targeting
Enzyme kinetics
Michaelis constant
(NAD(P)H:quinone reductase 2- and prodrug-based therapeutic systems, and cosubstrate preparation)

IT Polynucleotides
RL: BPR (Biological process); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)
(NAD(P)H:quinone reductase 2-encoding; NAD(P)H:quinone reductase 2- and prodrug-based therapeutic systems, and cosubstrate preparation)

IT Antibodies
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(conjugates, with NAD(P)H:quinone reductase 2; NAD(P)H:quinone reductase 2- and prodrug-based therapeutic systems, and cosubstrate preparation)

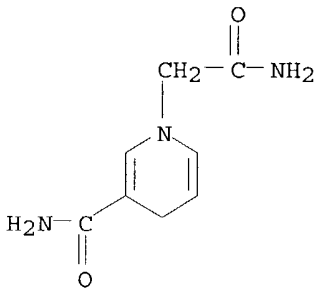
IT Neuroglia
(glioblastoma, inhibitors; NAD(P)H:quinone reductase 2- and prodrug-based therapeutic systems, and cosubstrate preparation)
IT Antitumor agents
(glioblastoma; NAD(P)H:quinone reductase 2- and prodrug-based therapeutic systems, and cosubstrate preparation)
IT Biological transport
(internalization; NAD(P)H:quinone reductase 2- and prodrug-based therapeutic systems, and cosubstrate preparation)
IT Drug delivery systems
(prodrugs; NAD(P)H:quinone reductase 2- and prodrug-based therapeutic systems, and cosubstrate preparation)
IT Neoplasm
(promoter specific for; NAD(P)H:quinone reductase 2- and prodrug-based therapeutic systems, and cosubstrate preparation)
IT Promoter (genetic element)
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(tumor-specific; NAD(P)H:quinone reductase 2- and prodrug-based therapeutic systems, and cosubstrate preparation)
IT **64881-21-6P** 114554-11-9P
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)
(NAD(P)H:quinone reductase 2- and prodrug-based therapeutic systems, and cosubstrate preparation)
IT 53-57-6, NADPH 58-68-4, NADH 4229-56-5, NMNH 9037-41-6, Nitroreductase
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(NAD(P)H:quinone reductase 2- and prodrug-based therapeutic systems, and cosubstrate preparation)
IT 952-92-1P 7145-37-1P 17750-23-1P 17750-24-2P 58880-44-7P 89080-16-0P 99362-74-0P 115503-79-2P 218443-91-5P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(NAD(P)H:quinone reductase 2- and prodrug-based therapeutic systems, and cosubstrate preparation)
IT 21919-05-1, CB 1954 21919-05-1D, CB 1954, analogs 667919-86-0
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(NAD(P)H:quinone reductase 2- and prodrug-based therapeutic systems, and cosubstrate preparation)
IT 119643-82-2
RL: BSU (Biological study, unclassified); MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative)
(NAD(P)H:quinone reductase 2- and prodrug-based therapeutic systems, and cosubstrate preparation)
IT 19132-12-8, Reduced nicotinamide riboside
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(cosubstrate; NAD(P)H:quinone reductase 2- and prodrug-based therapeutic systems, and cosubstrate preparation)
IT 19132-12-8D, Reduced nicotinamide riboside, analogs
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(cosubstrates; NAD(P)H:quinone reductase 2- and prodrug-based therapeutic systems, and cosubstrate preparation)
IT 5463-59-2P 51652-08-5P 52047-79-7P 72306-81-1P 97009-81-9P 106047-77-2P 109942-74-7P 126298-92-8P **218443-88-0P**

218443-90-4P 218443-92-6P 218443-93-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction; NAD(P)H:quinone reductase 2- and prodrug-based therapeutic systems, and cosubstrate preparation)

IT 75-03-6 75-26-3, 2-Bromopropane 75-30-9, 2-Iodopropane 98-92-0, Nicotinamide 100-39-0, Benzyl bromide 106-94-5, 1-Bromopropane 107-08-4, 1-Iodopropane 141-76-4, 3-Iodopropionic acid 144-48-9, 2-Iodoacetamide 624-76-0, 2-Iodoethanol 627-18-9, 3-Bromo-1-propanol 1120-71-4, 1,3-Propanesultone 6456-44-6 17376-04-4, (2-Iodoethyl)benzene
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction; NAD(P)H:quinone reductase 2- and prodrug-based therapeutic systems, and cosubstrate preparation)

IT **64881-21-6P**
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)
(NAD(P)H:quinone reductase 2- and prodrug-based therapeutic systems, and cosubstrate preparation)

RN 64881-21-6 HCAPLUS
CN 1(4H)-Pyridineacetamide, 3-(aminocarbonyl)- (9CI) (CA INDEX NAME)



L28 ANSWER 4 OF 11 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1985:418998 HCAPLUS
DN 103:18998
ED Entered STN: 27 Jul 1985
TI Deuterium isotope effects for the nonenzymic and glutamate dehydrogenase catalyzed reduction of an α-imino acid by NADH
AU Srinivasan, R.; Fisher, Harvey F.
CS Dep. Biochem., Univ. Kansas, Kansas City, MO, 64128, USA
SO Journal of the American Chemical Society (1985), 107(14), 4301-5
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA English
CC 7-4 (Enzymes)
Section cross-reference(s): 34
AB The mechanisms of the nonenzymic and glutamate dehydrogenase-catalyzed reduction of an α-imino acid, Δ1-pyrroline-2-carboxylic acid, by NAD(P)H were studied by deuterium isotope effects. The partition isotope effects for the nonenzymic reaction with 4-deuterated 1,4-dihydronicotinamides were about the same as the corresponding observed kinetic isotope effects with 4,4-dideuterio-1,4-dihydronicotinamides, suggesting that the H-transfer step is solely rate-limiting. This reaction was characterized by an intrinsic primary kinetic isotope effect

of 1.3 and a very product-like transition state. The enzymic reaction was studied by determining the 2nd-order rate consts. for the reduction of the imino acid by the enzyme-NADH complex with 4,4-dideuterio and stereospecifically labeled 4-deuterio NADH. The primary isotope effect when the in-place H atom was protium was 3.80, and the secondary isotope effect when the in-flight H atom was protium was 1.21. Deuteration at 1 site lowered the isotope effect at the other by 13%. The following conclusions emerged for the reduction of the imino acid by the enzyme-NADH complex: (1) the H-transfer step is at least rate-contributing, (2) the transition state for this reaction is more sym. than that of the nonenzymic reaction, (3) both C-4 H atoms of NADH participate in the reaction coordinate motion, and (4) there is some nuclear tunneling in the reaction coordinate. The kinetic isotope effect for the oxidation of proline and proline-2d by enzyme-NADP was 4.1.

ST pyrrolinecarboxylate redn dihydronicotinamide isotope effect; glutamate dehydrogenase pyrrolinecarboxylate redn isotope effect

IT Kinetics, enzymic
(of glutamate dehydrogenase)

IT Reduction
(of pyrroline carboxylic acid by dihydronicotinamide, mechanism of)

IT Kinetics of reduction
(of pyrroline carboxylic acid, by dihydronicotinamide)

IT Isotope effect
(on pyrroline carboxylic acid enzymic and nonenzymic reduction, of deuterium)

IT 2139-03-9
RL: BIOL (Biological study)
(enzymic and nonenzymic reduction of, deuterium isotopes effects in)

IT 7782-39-0, biological studies
RL: PRP (Properties)
(isotope effect of, on pyrroline carboxylic acid enzymic and nonenzymic reduction)

IT 17750-27-5 60172-94-3 60764-22-9 **96555-70-3**
RL: BIOL (Biological study)
(pyrroline carboxylic acid reduction by, deuterium isotope effects in)

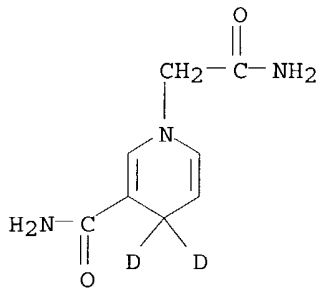
IT 58-68-4D, glutamate dehydrogenase complexes 10012-96-1D, glutamate dehydrogenase complexes 10021-11-1D, glutamate dehydrogenase complexes 60764-22-9D, glutamate dehydrogenase complexes
RL: RCT (Reactant); RACT (Reactant or reagent)
(pyrroline carboxylic acid reduction by, kinetics of)

IT 9029-12-3
RL: PRP (Properties)
(reaction kinetics of, with pyrroline carboxylic acid, deuterium isotope effects on)

IT **96555-70-3**
RL: BIOL (Biological study)
(pyrroline carboxylic acid reduction by, deuterium isotope effects in)

RN 96555-70-3 HCAPLUS

CN 1(4H)-Pyridine-4,4-d2-acetamide, 3-(aminocarbonyl)- (9CI) (CA INDEX NAME)



L28 ANSWER 5 OF 11 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1985:20200 HCAPLUS
DN 102:20200
ED Entered STN: 26 Jan 1985
TI Polymer-bound flavins. III. Effects of coil dimension and substrate structure on reaction kinetics in water/2-propanol mixtures
AU Bootsma, Jan P. C.; Rupert, Leo A. M.; Challa, Ger; Mueller, Franz
CS Lab. Polym. Chem., State Univ. Groningen, Groningen, 9747 AG, Neth.
SO Journal of Polymer Science, Polymer Chemistry Edition (1984), 22(9), 2169-80
CODEN: JPLCAT; ISSN: 0449-296X
DT Journal
LA English
CC 7-3 (Enzymes)
Section cross-reference(s): 36
AB The strong influence of medium composition (H2O/2-propanol mixts.) on the rate of oxidation of 1-substituted dihydronicotinamides by a flavin-containing polyelectrolyte was studied. The coil dimensions of the corresponding copolymer of styrene and vinylbenzyltriethylammonium chloride without flavin groups dramatically depend on the solvent. Viscometric measurements revealed compact coil conformations in solvents of both high H2O and high 2-propanol content, but pronounced coil expansion in intermediate mixts. These changes of polyelectrolyte coil dimensions are related to changes in electrostatic potential of the microreactors. Addition of 2-propanol also results in a decrease of substrate enrichments, caused by weakening of nonpolar polymer-substrate interactions, as was demonstrated for 1-carbamoylmethyl-, 1-benzyl-, and 1 decyl-substituted 1,4-dihydronicotinamide substrates. The enormous decrease in rate constant for oxidation of 1-decyl-1,4-dihydronicotinamide by flavin bound to styrene vinylbenzyltriethylammonium chloride copolymer upon increasing the 2-propanol content from 10 to 40% (volume/volume), from k = 3120 to 21 M-1 s-1, can thus be explained as a cooperation of both effects. Evidence for the formation of a charge-transfer complex between the polyelectrolyte-bound flavin and the dihydronicotinamide having a long-wavelength absorption is also presented.
ST polymer bound flavin dihydronicotinamide oxidn; solvent effect polymer bound flavin
IT Chains, chemical
(conformation of, of styrene copolymer, 2-propanol aqueous mixture effect on,
dihydronicotinamide oxidation by polymer-bound flavin in relation to)
IT Kinetics of oxidation
(of dihydronicotinamide derivs., by styrene copolymer-bound flavin, solvent effect in relation to)
IT Molecular association

(of styrene copolymer-bound flavin and dihydronicotinamide, dihydronicotinamide oxidation and formation of charge-transfer complex in relation to)

IT 32561-90-3D, reaction products with styrene-monobenzyltriethylammonium chloride copolymer
RL: RCT (Reactant); RACT (Reactant or reagent)
(dihydronicotimamide derivative reduction by, solvent effect in relation to)

IT 121-44-8D, reaction products with styrene copolymer containing bound flavin
29464-22-0D, reaction products with flavin and triethylamine
RL: BIOL (Biological study)
(dihydronicotinamide derivative reduction by, kinetics of, solvent effect in relation to)

IT 67-63-0, uses and miscellaneous
RL: USES (Uses)
(kinetics of oxidation of dihydronicotinamide derivs. by polymer-bound flavins in presence of aqueous)

IT 952-92-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(oxidation of, by styrene copolymer-bound flavin, solvent effect in relation to)

IT **64881-21-6P** 93674-24-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and oxidation by styrene copolymer-bound flavin, solvent effect in relation to)

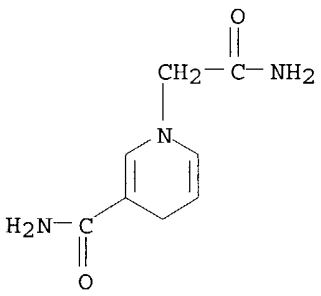
IT 35041-49-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)

IT 98-92-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with decyl iodide)

IT 2050-77-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with nicotinamide)

IT **64881-21-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and oxidation by styrene copolymer-bound flavin, solvent effect in relation to)

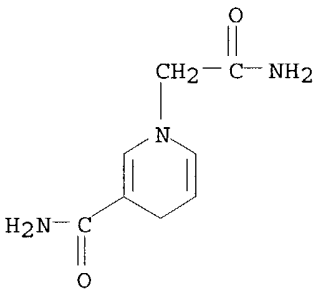
RN 64881-21-6 HCAPLUS
CN 1(4H)-Pyridineacetamide, 3-(aminocarbonyl)- (9CI) (CA INDEX NAME)



L28 ANSWER 6 OF 11 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1982:64792 HCAPLUS

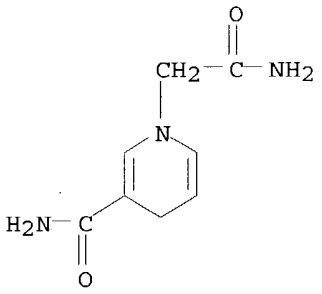
DN 96:64792
ED Entered STN: 12 May 1984
TI The pyridinium-dihydropyridine system. Reduction potentials and the mechanism of oxidation of 1,4-dihydropyridines by a Schiff base
AU Srinivasan, R.; Medary, Richard T.; Fisher, Harvey F.; Norris, Donald J.; Stewart, Ross
CS Sch. Med., Univ. Kansas, Kansas City, MO, 64128, USA
SO Journal of the American Chemical Society (1982), 104(3), 807-12
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA English
CC 7-4 (Enzymes)
AB As a model system for the glutamate dehydrogenase-catalyzed reductive amination of α-ketoglutarate, the reduction of a Schiff base, Δ1-pyrroline-2-carboxylic acid, was studied with a series of 14 N-1- and C-3-substituted, 1,4-dihydropyridines, including NMNH, NADH, and NADPH. The reversible electrode potentials of 8 of the dihydropyridines, all dihydronicotinamides, were also determined The reduction reaction had the following characteristics: (a) it was 1st-order in protonated Schiff base (zwitterionic form) and 1st-order in the dihydropyridine; (b) there was a small deuterium isotope effect when the C-4 position of the dihydropyridine was deuterated (1.20-1.57 at 25°); (c) there was a direct transfer of H from C-4 of the dihydropyridine to C-2 of the pyrroline; (d) the rates for 7 N-1-substituted dihydronicotinamides were correlated satisfactorily with σ* giving ρ* = -1.98 (H2O) and -1.78 (aqueous MeOH), there being only a modest difference in rates in these 2 solvents; (e) there was a good correlation between the rates of reduction by the dihydronicotinamides and the E0 values of the reversible 2-electron dihydropyridine-pyridinium couple, the effect being 31.0 mV per logarithmic unit of rate; (f) there was a close correlation between the rates of reduction of pyrroline and of flavin by the dihydropyridines; and (g) the enthalpy and entropy of activation for the rate-controlling step in the reduction by 1-benzyl-1,4-dihydronicotinamide were, resp., 15.7 kcal/mol and -7.6 entropy units. Apparently, direct hydride transfer took place to produce proline in a single step and it could be inferred that the transition state closely resembled the products in structure. The similarity between pyrroline and flavin reduction suggested that the latter reaction may also be a direct hydride transfer.
ST glutamate dehydrogenase model; dihydropyridine oxidn Schiff base mechanism; redox potential dihydropyridine deriv; pyrrolinecarboxylate redn dihydropyridine kinetics
IT Isotope effect
(of deuterium, in pyrrolinecarboxylate reduction by dihydropyridines)
IT Kinetics of reduction
(of pyrrolinecarboxylate by dihydropyridines)
IT Substituent constant
(Hammett, of dihydropyridines, in pyrrolinecarboxylate reduction)
IT Electric potential
(redox, of dihydropyridines)
IT 80028-67-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with dihydropyridines)
IT 53-57-6 58-68-4 952-92-1 4229-56-5 7145-37-1 17750-23-1 53164-23-1 64881-16-9 64881-17-0 64881-18-1 64881-20-5 **64881-21-6** 64881-22-7 64881-23-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(pyrrolinecarboxylate reduction by, kinetics of)
IT 9029-12-3
RL: MSC (Miscellaneous); PRP (Properties)

(reaction mechanism of, models for)
IT 2139-03-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction of, with dihydropyridines, as glutamate dehydrogenase model)
IT **64881-21-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(pyrrolinecarboxylate reduction by, kinetics of)
RN 64881-21-6 HCAPLUS
CN 1(4H)-Pyridineacetamide, 3-(aminocarbonyl)- (9CI) (CA INDEX NAME)



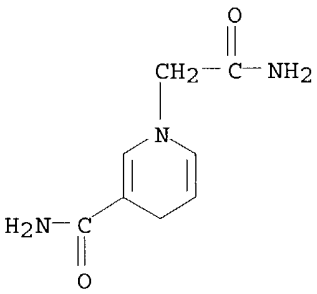
L28 ANSWER 7 OF 11 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1981:3504 HCAPLUS
DN 94:3504
ED Entered STN: 12 May 1984
TI The reduction of aryl trifluoromethyl ketones by N-carbamoylmethyl-1,4-dihydronicotinamide
AU Stewart, Ross; Teo, K. C.; Ng, L. K.
CS Dep. Chem., Univ. British Columbia, Vancouver, BC, V6T 1Y6, Can.
SO Canadian Journal of Chemistry (1980), 58(23), 2497-503
CODEN: CJCHAG; ISSN: 0008-4042
DT Journal
LA English
CC 22-5 (Physical Organic Chemistry)
AB The reaction of 15 aryl trifluoromethyl ketones with N-(carbamoylmethyl)-1,4-dihydronicotinamide (I) was studied in aqueous sulfolane buffer. The unsubstituted ketone and those containing electron-withdrawing groups in the ring have the following reaction characteristics: (a) a high yield of alc. is obtained, (b) the observed reaction rate is independent of ring substituent; however, when corrections are made for the degree of hydration of the ketones the rate correlates with Hammett σ values with ρ = +1.98, (c) a secondary isotope effect of .apprx.1.08 and primary isotope effects of 1.45-1.62 are observed at 43.4° for the reaction of I containing 1 or 2 D atoms at C-4, (d) ΔH.thermod. = 15.2 kcal mol-1 and ΔS.thermod. = -27.0 cal deg-1 mol-1 for the unsubstituted compound, uncorrected for ketone hydration; ΔS.thermod. for reaction of the unhydrated ketone and I is estimated as -45 to -50 cal deg-1 mol-1. The reduction mechanism is consistent with hydride transfer from I to the ketone, very possibly accompanied by blind-alley formation of an adduct between ketone hydrate and I. Ketones containing electron-donating groups in the ring react with I in some undetd. way, giving little or no alc. as product.
ST redn aryl trifluoromethyl ketone mechanism; nicotinamide carbamoylmethyldihydro redn ketone kinetics
IT Kinetics of reduction
(of aryl trifluoromethyl ketones with (carbamoylmethyl)dihydronicotinam

ide)
IT Reduction
(of aryl trifluoromethyl ketones with (carbamoylmethyl)dihydronicotinamide, mechanism of)
IT Ketones, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(aryl trifluoromethyl, reduction of, with (carbamoylmethyl)dihydronicotinamide, kinetics of)
IT **64881-21-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction of aryl trifluoromethyl ketones with)
IT 321-31-3 321-37-9 394-59-2 434-45-7 655-32-3 657-15-8 708-64-5 711-38-6 721-37-9 2396-05-6 16184-89-7 23516-79-2 73471-96-2 73471-97-3 75822-10-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction of, with (carbamoylmethyl)dihydronicotinamide, kinetics of)
IT **64881-21-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction of aryl trifluoromethyl ketones with)
RN 64881-21-6 HCAPLUS
CN 1(4H)-Pyridineacetamide, 3-(aminocarbonyl)- (9CI) (CA INDEX NAME)

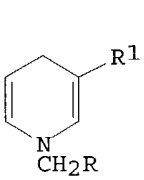


L28 ANSWER 8 OF 11 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1980:180442 HCAPLUS
DN 92:180442
ED Entered STN: 12 May 1984
TI Substituent effects in the reduction of trifluoroacetophenones by a dihydronicotinamide
AU Stewart, Ross; Ng, L. K.; Teo, K. C.
CS Dep. Chem., Univ. British Columbia, Vancouver, BC, V6T 1W5, Can.
SO Tetrahedron Letters (1979), (33), 3061-4
CODEN: TELEAY; ISSN: 0040-4039
DT Journal
LA English
CC 22-8 (Physical Organic Chemistry)
AB The reduction rates of m- and p-RC6H4COCF3 (R = electron withdrawing group) to the corresponding alcs. by N-carbamoylmethyl-3-carbamoyl-1,4-dihydropyridine correlate closely with the equilibrium consts. for hydration of the same compds. High yields of RC6H4CH(OH)CF3 were obtained when electron donating substituents were absent from the ring.
ST fluoroacetophenone redn nicotinamide kinetics; LFER redn fluoroacetophenone nicotinamide; acetophenone fluoro redn nicotinamide kinetics; substituent effect redn fluoroacetophenone nicotinamide
IT Linear free energy relationship
(for dihydronicotinamide derivative reduction vs. hydration of

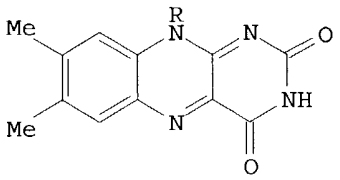
trifluoroacetophenones)
IT Kinetics of reduction
(of trifluoroacetophenones, by dihydronicotinamide)
IT Reduction
(of trifluoroacetophenones, by dihydronicotinamide, substituent effect on)
IT Substituent effect
(on reduction of trifluoroacetophenones by dihydronicotinamide)
IT **64881-21-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction by, of trifluoroacetophenones, substituent effect on)
IT 711-38-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction of, by dihydronicotinamide derivative)
IT 321-31-3 321-37-9 394-59-2 434-45-7 655-32-3 657-15-8 708-64-5 721-37-9 16184-89-7 73471-96-2 73471-97-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction of, by dihydronicotinamide derivative, substituent effect in)
IT **64881-21-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction by, of trifluoroacetophenones, substituent effect on)
RN 64881-21-6 HCAPLUS
CN 1(4H)-Pyridineacetamide, 3-(aminocarbonyl)- (9CI) (CA INDEX NAME)



L28 ANSWER 9 OF 11 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1978:441983 HCAPLUS
DN 89:41983
ED Entered STN: 12 May 1984
TI The pyridinium-dihydropyridine system. Part 2. Substituent effects on the oxidation of 1,4-dihydropyridines by flavins
AU Stewart, Ross; Norris, Donald J.
CS Dep. Chem., Univ. Br. Columbia, Vancouver, BC, Can.
SO Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1972-1999) (1978), (3), 246-9
CODEN: JCPKBH; ISSN: 0300-9580
DT Journal
LA English
CC 22-5 (Physical Organic Chemistry)
Section cross-reference(s): 33
GI



I



II

AB The kinetics of oxidation of dihydropyridines I (R = H, CH2OH, OMe, COMe, R1 = CONH2; R = CONH2, R1 = COMe) and I (R = CO2Me, CN, CONH2, R1 = CONH2; R = CONH2, R1 = CN) to pyridinium derivs. by flavins II (R = ribityl) and II (R = ribityl phosphate), resp., showed that R1 in I has a greater effect on the reaction rate than R. Oxidation rates of I (R1 = CONH2, R as above except OMe) correlated linearly with σ*.

ST carbamoylpyridine oxidn flavin nucleotide; pyridine carbamoyl oxidn riboflavin kinetics

IT Reaction constant
(for oxidation of carbamoyldihydropyridines by riboflavin)

IT Substituent effect
(in oxidation of carbamoyldihydropyridine derivs. by riboflavin)

IT Kinetics of oxidation
(of carbamoyldihydropyridine derivs. by riboflavin, substituent effect in relation to)

IT Nucleotides, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(oxidation by, of dihydropyridines, kinetics of)

IT 83-88-5, reactions 146-17-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(oxidation by, of dihydropyridines, kinetics of)

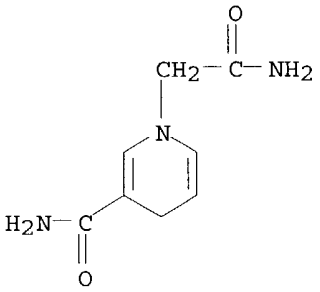
IT 58-68-4 4229-56-5 7145-37-1 17750-23-1 53164-23-1 64881-17-0 64881-18-1 64881-20-5 **64881-21-6** 64881-22-7 64881-23-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(oxidation of, by riboflavin, substituent effect in relation to kinetics of)

IT 3106-60-3P 66822-21-7P 66822-22-8P 66822-23-9P 66822-24-0P 66822-25-1P **66822-26-2P** 66822-27-3P 66822-28-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by oxidation of dihydropyridine derivative with flavin)

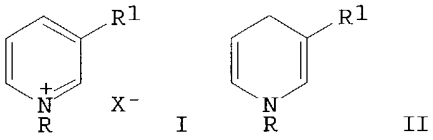
IT **64881-21-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(oxidation of, by riboflavin, substituent effect in relation to kinetics of)

RN 64881-21-6 HCAPLUS

CN 1(4H)-Pyridineacetamide, 3-(aminocarbonyl)- (9CI) (CA INDEX NAME)

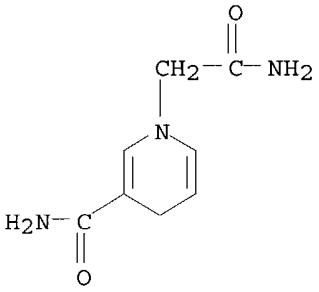


L28 ANSWER 10 OF 11 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1978:6668 HCAPLUS
DN 88:6668
ED Entered STN: 12 May 1984
TI The pyridinium-dihydropyridine system. I. Synthesis of a series of substituted pyridinium ions and their 1,4-dihydro reduction products and a determination of their stabilities in aqueous buffers
AU Norris, Donald J.; Stewart, Ross
CS Dep. Chem., Univ. British Columbia, Vancouver, BC, Can.
SO Canadian Journal of Chemistry (1977), 55(10), 1687-95
CODEN: CJCHAG; ISSN: 0008-4042
DT Journal
LA English
CC 27-17 (Heterocyclic Compounds (One Hetero Atom))
GI



AB Fourteen pyridinium salts (I, R = CH2CO2-, R1 = CONH2, X = -; R = Me, R1 = CONH2, X = I; R = CH2CONH2, R1 = CN, X = Cl; etc.) and the 1,4-dihydro derivs. (II) were prepared and their stabilities determined in aqueous acetate and tris(hydroxymethyl)aminomethane (Tris) buffers. The pyridinium ions are stable in acidic solution but undergo either ring attack or amide or ester hydrolysis under basic conditions, whereas the dihydropyridines undergo covalent hydration in acid solution For only 4 pairs of compds. and one buffer system (Tris) are there pH-ranges in which the pyridinium and dihydropyridine forms are simultaneously stable (less than 10% decomposition in 24 h). These compds. have a carbamoyl or acetyl group at the 3-position and either a CH2OMe, CH2COMe, CH2CONH2 group at the 1-position. The HOAc-catalyzed rates of hydration of the 1-alkyl-3-carbamoyl-1,4-dihydropyridines are correlated by σ* values with a ρ* of -2.00, consistent with protonation being the rate-controlling step.
ST pyridinium; stability pyridinium; dihydropyridine stability; pyridine dihydro stability
IT Kinetics of hydration
(of 1-alkyl-3-carbamoyl-1,4-dihydropyridine in acid buffers)
IT Stability

(of pyridinium salts and dihydropyridine in aqueous buffers)
IT Reduction
(of pyridinium, hydropyridines from)
IT 7145-37-1P 17750-23-1P 53164-23-1P 64881-16-9P 64881-17-0P
64881-18-1P 64881-19-2P 64881-20-5P **64881-21-6P**
64881-22-7P 64881-23-8P 64881-24-9P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and stability of)
IT 6456-44-6P 7145-36-0P 37928-74-8P 41220-29-5P 53164-19-5P
64881-07-8P 64881-08-9P 64881-09-0P 64881-10-3P **64881-11-4P**
64881-12-5P 64881-13-6P 64881-14-7P 64881-15-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, reduction, and stability of)
IT **64881-21-6P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and stability of)
RN 64881-21-6 HCAPLUS
CN 1(4H)-Pyridineacetamide, 3-(aminocarbonyl)- (9CI) (CA INDEX NAME)



L28 ANSWER 11 OF 11 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1973:84204 HCAPLUS
DN 78:84204
ED Entered STN: 12 May 1984
TI Synthesis and chelating properties of carboxylic derivatives of piperidine and piperazine
AU Piotrowska, Hanna; Serafinowa, Barbara; Trybulowa, Zofia; Wejroch-Matacz, Krystyna; Boguszewska, Zofia
CS Polytech. Warsaw, Warsaw, Pol.
SO Roczniki Chemii (1972), 46(10), 1777-88
CODEN: ROCHAC; ISSN: 0035-7677
DT Journal
LA Polish
CC 27-17 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 28
GI For diagram(s), see printed CA Issue.
AB Fifty compds. I, II, III, IV, and V [X and Y = NHNH2, NH2, OH, and OEt; Z = CH2COX, CH(COX)2] were prepared, in most cases by routine methods from the corresponding esters, and tested for chelating properties (Cu, Hg, Pb, Fe, Sr, and Ca ions). Best chelation effects with Mg and Fe ions were observed with dihydrazides of I and II and with tetrahydrazides V. Similarly, diamide and dimethylamide I and tetraamide V formed sparingly soluble complexes with Fe ions. In general, derivs. of malonic acid showed interesting chelating properties.
ST piperidines piperazines chelation; copper piperidines chelation; mercury

piperidines chelation; lead piperidines chelation; iron piperidines chelation; strontium piperidines chelation; calcium piperidines chelation

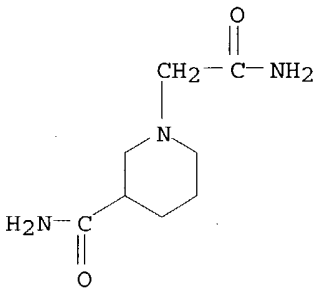
IT Chelation
(of piperidine and piperazine derivs. with metal ions)

IT 1,2-Piperidinediacetic acid, sodium salt, metal complexes
1,3-Piperidinediacetic acid, sodium salt, metal complexes
1,4-Piperazinediacetic acid, sodium salt, metal complexes
1,4-Piperazinediacetic acid, α,α'-dicarboxy-, sodium salt, metal complexes
1,4-Piperidinediacetic acid, sodium salt, metal complexes
1-Piperidineacetic acid, 2-carboxy-, sodium salt, metal complexes
1-Piperidineacetic acid, 3-carboxy-, sodium salt, metal complexes
Calcium, ionic complexes with piperidine and piperazine derivative
Copper, ionic complexes with piperidine and piperazine derivative
Iron, ionic complexes with piperidine and piperazine derivative
Lead, ionic complexes with piperidine and piperazine derivative
Mercury, ionic complexes with piperidine and piperazine derivative
Strontium, ionic complexes with piperidine and piperazine derivative
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT 4711-17-5 5430-78-4 22277-84-5 40479-09-2 40479-10-5 40479-12-7
40479-13-8 40479-14-9 40479-15-0 **40479-16-1** 40479-17-2
40479-18-3 40479-19-4 40479-20-7 40479-21-8 40479-22-9
40479-23-0 40479-24-1 40479-25-2 40479-26-3 40479-27-4
40479-28-5 40479-29-6 40479-30-9 40479-31-0 40479-32-1
40479-33-2 40479-34-3 40479-35-4 40479-36-5 40479-37-6
40479-38-7 40479-39-8 40479-40-1 40479-41-2 40479-42-3
40479-43-4 40479-44-5 40479-45-6 40479-46-7 40479-47-8
40479-48-9 40479-50-3 40479-52-5 40479-53-6 40479-54-7
40479-55-8 40479-56-9 40531-37-1 40531-38-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(chelation of)

IT **40479-16-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(chelation of)

RN 40479-16-1 HCAPLUS
CN 1-Piperidineacetamide, 3-(aminocarbonyl)- (9CI) (CA INDEX NAME)



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FILE 'HOME' ENTERED AT 16:52:18 ON 15 JUL 2004

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PASSWORD:
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FILE 'HOME' ENTERED AT 16:48:18 ON 15 JUL 2004

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FILE 'HCAPLUS' ENTERED AT 16:49:40 ON 15 JUL 2004
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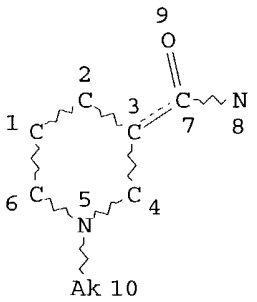
FILE COVERS 1907 - 15 Jul 2004 VOL 141 ISS 3
FILE LAST UPDATED: 14 Jul 2004 (20040714/ED)

This file contains CAS Registry Numbers for easy and accurate
substance identification.

'OBI' IS DEFAULT SEARCH FIELD FOR 'HCAPLUS' FILE

=> d que l42
L17 STR



NODE ATTRIBUTES:
CONNECT IS X3 RC AT 8
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC 5
NUMBER OF NODES IS 10

STEREO ATTRIBUTES: NONE
L19 1422 SEA FILE=REGISTRY SSS FUL L17
L29 487 SEA FILE=HCAPLUS ABB=ON PLU=ON L19
L41 215 SEA FILE=HCAPLUS ABB=ON PLU=ON L29 AND P/DT
L42 101 SEA FILE=HCAPLUS ABB=ON PLU=ON L41 AND (PY<=1997 OR PRY<=1997 OR AY<=1997)

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L42 ANSWER 1 OF 101 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:552324 HCAPLUS
DN 137:109488
ED Entered STN: 25 Jul 2002
TI Preparation of peptidyl calcium channel blockers
IN Booth, Richard John; Brogley, Louis; Cody, Wayne Livingston; Connor, David Thomas; Hamilton, Harriet Wall; He, John Xiaoqiang; Hu, Lain-Yen; Lescosky, Leonard Joseph; Malone, Thomas Charles; Nadasdi, Laszlo; Rafferty, Michael Francis; Roth, Bruce David; Silva, Diego F.; Song, Yuntao; Szoke, Balazs G.; Urge, Laszlo
PA Warner-Lambert Company, USA; Neurex Corporation
SO U.S., 86 pp.
CODEN: USXXAM
DT **Patent**
LA English
IC ICM A61K038-05
ICS C07K005-06
NCL 514019000
CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 1, 63
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 6423689	B1	20020723	US 1998-212785	19981216 <--
PRAI US 1997-68485P	P	19971222 <--		

OS MARPAT 137:109488
AB Peptides R5CONHCR1R7CONHCR2(CH2-p-C6H4-Y-R4)COR3 [R1 = alkyl, benzyl, H, indolylmethyl, Q-(CH2)n (Q = alkylthio, substituted Ph, cycloalkyl, heteroaryl; n = 0-5); R2 = H, alkyl; R3 = alkoxy, Ph(CH2)nO, NH2, alkylamino, cycloalkyl, etc.; R4 = Q(CH2)n, where Q = (un)substituted Ph, NH2, dialkylamino, pyridyl, etc.; R5 = N(CH2)m (m = 2-7); R7 = H, alkyl; Y = O, NR4, NH, absent, CH:CH, C.tplbond.C] or their pharmaceutically acceptable salts, esters, amides, and prodrugs were prepared as calcium channel blockers. Pharmaceutical compns. containing these compds. can be used to treat stroke, cerebral ischemia, head trauma, or epilepsy. Thus, [S-(R*,R*)]-2-[2-[(azepane-1-carbonyl)amino]-4-methylpentanoylamino]-3-(4-benzyloxy-phenyl)propionic acid tert-Bu ester was prepared via amidation reaction and showed IC50 = 0.35 μM for inhibition of calcium flux in IMR-32 cells and protected 5/5 mice from tonic convulsions at 30 mg/kg at 15 min posttreatment time. The syntheses of 271 compds. of the invention are described in the examples and > 200 addnl. compds. are given in the claims.
ST peptide prepn calcium channel blocker; antiepileptic peptide prepn calcium channel blocker
IT Ion channel blockers
(calcium; preparation of peptidyl calcium channel blockers)

IT Brain, disease
(ischemia; preparation of peptidyl calcium channel blockers)
IT Analgesics
Anticonvulsants
Epilepsy
Human
Pain
(preparation of peptidyl calcium channel blockers)
IT Dipeptides
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of peptidyl calcium channel blockers)
IT Brain, disease
(stroke; preparation of peptidyl calcium channel blockers)
IT Head, disease
(trauma; preparation of peptidyl calcium channel blockers)
IT 225925-09-7P 225925-12-2P 443689-91-6P 443689-92-7P 443689-93-8P
443689-94-9P 443689-95-0P 443689-96-1P 443689-97-2P 443689-98-3P
443689-99-4P 443690-00-4P 443690-01-5P 443690-02-6P 443690-03-7P
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443692-27-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of peptidyl calcium channel blockers)

IT 443692-28-2P 443692-29-3P 443692-30-6P 443692-31-7P 443692-32-8P
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RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of peptidyl calcium channel blockers)

IT 50-01-1, Guanidine hydrochloride 51-45-6, Histamine, reactions 51-67-2, Tyramine 59-67-6, Nicotinic acid, reactions 60-18-4, Tyrosine, reactions 61-54-1, Tryptamine 75-64-9, tert-Butylamine, reactions 75-98-9, Pivalic acid 76-05-1, Trifluoroacetic acid, reactions 78-27-3, 1-Ethynyl 1-cyclohexanol 79-09-4, Propionic acid, reactions 79-31-2, Isobutyric acid 86-84-0, 1-Naphthyl isocyanate 87-51-4, Indole-3-acetic acid, reactions 91-21-4, 1,2,3,4-Tetrahydroisoquinoline 92-54-6, n-Phenylpiperazine 96-20-8, 2-Amino-1-butanol 96-50-4, 2-Aminothiazole 98-16-8, 3-Trifluoromethylaniline 98-58-8, 4-Bromophenylsulfonyl chloride 98-68-0 98-74-8, 4-Nitrobenzenesulfonyl chloride 99-92-3 99-98-9, N,N-Dimethyl-p-phenylenediamine 100-07-2, 4-Methoxybenzoyl chloride 100-28-7, 4-Nitrophenyl isocyanate 100-46-9, Benzylamine, reactions 100-55-0, 3-Pyridylcarbinol 102-36-3, 3,4-Dichlorophenyl isocyanate 103-71-9, Phenyl isocyanate, reactions 103-76-4, N-(2-Hydroxyethyl)piperazine 104-10-9, 4-Aminophenethyl alcohol 104-12-1, 4-Chlorophenyl isocyanate 104-63-2, N-Benzylethanolamine 104-81-4, α-Bromo-p-xylene 104-94-9, p-Anisidine 106-40-1, 4 Bromoaniline 107-92-6, Butyric acid, reactions 108-00-9, n,n-Dimethylethylenediamine 108-15-6, 1-Dimethylamino-2-propylamine 109-01-3, n-Methylpiperazine 109-90-0, Ethyl isocyanate 110-89-4, Piperidine, reactions 110-91-8, Morpholine, reactions 111-26-2, Hexylamine 111-36-4, Butyl isocyanate 111-41-1, 2-(2-Aminoethylamino)ethanol 111-49-9 115-70-8, 2-Amino-2-ethyl-1,3-propanediol 122-80-5, 4'-Aminoacetanilide 123-90-0, Thiomorpholine 124-68-5, 2-Amino-2-methyl-1-propanol 133-59-5, o-Toluenesulfonyl chloride 139-59-3, 4-Phenoxyaniline 141-43-5, reactions 141-91-3, 2,6-Dimethylmorpholine 151-18-8, 3-Aminopropionitrile 156-87-6, 3-Amino-1-propanol 288-13-1, Pyrazole 327-78-6, 4-Chloro-3-(trifluoromethyl)phenyl isocyanate 329-01-1 349-88-2 356-42-3, Pentafluoropropionic anhydride 403-43-0, 4-Fluorobenzoyl chloride 462-08-8, 3-Aminopyridine 505-66-8, Homopiperazine 527-69-5, 2-Furoyl chloride 534-03-2, Serinol 536-74-3, Phenyl acetylene 539-48-0, p-Xylylenediamine 556-61-6, Methyl isothiocyanate 586-95-8, 4-Pyridylcarbinol 586-98-1, 2-Pyridylcarbinol 591-27-5, 3-Hydroxyaniline 592-82-5, Butyl isothiocyanate 598-74-3, 1,2-Dimethylpropylamine 605-65-2, Dansyl chloride 614-68-6, o-Tolyl isocyanate 616-29-5, 1,3-Diamino-2-propanol 617-89-0, Furfurylamine 622-58-2, p-Tolyl isocyanate 622-59-3, p-Tolyl

isothiocyanate 624-83-9, Methyl isocyanate 626-56-2, 3-Methylpiperidine 658-48-0, α-Methyltyrosine 694-05-3, 1,2,3,6-Tetrahydropyridine 696-40-2, 3-Iodobenzylamine 700-87-8, 2-Methoxyphenyl isocyanate 705-21-5, 3,5-Dichlorobenzenesulfonyl chloride 765-30-0, Cyclopropylamine 824-94-2, 4-Methoxybenzyl chloride 830-96-6, 3-Indolepropionic acid 841-77-0 879-65-2, 2-Quinoxaline carboxylic acid 917-92-0, 3,3-Dimethylbutyne 931-48-6, Cyclohexylethyne 962-39-0, Phenylalanine benzyl ester 1016-19-9, 3,4,5-Trimethoxyphenyl isocyanate 1121-46-6, 2-Furanethanamine 1122-82-3, Cyclohexyl isothiocyanate 1136-45-4, 5-Methyl-3-phenylisoxazole-4-carboxylic acid 1548-13-6, 4-Trifluoromethylphenyl isocyanate 1632-84-4, 4-(Methylthio)phenyl isocyanate 1710-98-1, 4-tert-Butylbenzoyl chloride 1711-05-3, 3-Methoxybenzoyl chloride 1738-68-7 1738-69-8 1795-48-8, Isopropyl isocyanate 1828-66-6, 4-Morpholinesulfonyl chloride 1918-77-0, Thiophene-2-acetic acid 1945-84-2, 2-Ethynylpyridine 1985-12-2, Benzene, 1-bromo-4-isothiocyanato- 2038-03-1, 4-Morpholineethanamine 2130-96-3 2217-40-5, 1,2,3,4-Tetrahydro-1-naphthylamine 2243-83-6, 2-Naphthoyl chloride 2252-63-3, 1-(4-Fluorophenyl)piperazine 2359-60-6, 4-Piperidinoaniline 2488-15-5 2493-02-9, 4-Bromophenyl isocyanate 2516-47-4, Aminomethylcyclopropane 2550-36-9, Bromomethylcyclohexane 2612-57-9, 2,4-Dichlorophenyl isocyanate 2620-50-0, Piperonylamine 2706-56-1, 2-(2-Aminoethyl)pyridine 2740-81-0, 2-Chlorophenyl isothiocyanate 2759-28-6, 1-Benzylpiperazine 2909-38-8, 3-Chlorophenyl isocyanate 3096-71-7 3173-53-3, Cyclohexyl isocyanate 3173-56-6, Benzyl isocyanate 3218-02-8, Aminomethylcyclohexane 3312-60-5, n 3 Amino propyl cyclohexylamine 3320-83-0, 2-Chlorophenyl isocyanate 3367-95-1 3535-37-3, 3,4-Dimethoxybenzoyl chloride 3731-53-1, 4-Pyridinemethanamine 3978-80-1 4152-09-4, N-Benzylethylenediamine 4411-26-1, 1-Adamantylisothiocyanate 4521-61-3, 3,4,5-Trimethoxybenzoyl chloride 4572-03-6 4606-65-9, 3-Piperidinemethanol 4897-50-1, 4-Piperidinopiperidine 5036-48-6, 1-(3-Aminopropyl)imidazole 5308-25-8, N-Ethylpiperazine 5382-16-1, 4-Hydroxypiperidine 5416-93-3, 4-Methoxyphenyl isocyanate 5452-35-7, Cycloheptylamine 6419-36-9, 3-Pyridylacetic acid hydrochloride 6859-99-0, 3-Hydroxypiperidine 7087-68-5 7144-05-0, 4-Aminomethylpiperidine 7154-73-6, 1-Pyrrolidineethanamine 7223-38-3, 1-Dimethylamino 2-propyne 7356-00-5, Bis(2-aminopropyl)amine 7568-93-6, 2-Amino-1-phenylethanol 10442-03-2 13139-15-6 13349-82-1 13889-98-0, 1-Acetylpiperazine 13952-84-6, sec-Butylamine 14002-51-8, 4-Biphenylcarbonyl chloride 15084-51-2, 4-tert-Butylphenylsulfonyl chloride 15159-40-7, 4-Morpholinecarbonyl chloride 15674-67-6, 3-(Diethylamino)propionic acid hydrochloride 15761-39-4 16331-46-7, 4-Ethoxybenzoyl chloride 16369-05-4, Valinol 16588-74-2, 3,5-Bistrifluoromethylphenyl isocyanate 16629-19-9, 2-Thiophenesulfonyl chloride 16874-12-7, L-Tyrosine, 1,1-dimethylethyl ester 17201-43-3, α-Bromo p tolunitrile 17831-01-5 18908-07-1, 3-Methoxyphenyl isocyanate 19241-24-8 21169-71-1, Isoxazole-5-carboxylic acid 21615-34-9, 2-Methoxybenzoyl chloride 22300-56-7 23159-07-1, 3-Pyrrolidinopropylamine 24313-88-0, 3,4,5-Trimethoxyaniline 24935-08-8 25054-53-9, 1,3-Benzodioxole-5-carbonyl chloride 25560-00-3 27578-60-5, 1 2 Aminoethyl piperidine 28143-91-1 28556-81-2, 2,6-Dimethylphenyl isocyanate 30806-83-8 31252-42-3, 4-Benzylpiperidine 33375-06-3, (R)-(+)-.α.-Methylbenzyl isocyanate 34893-92-0, 3,5-Dichlorophenyl isocyanate 35019-96-6, trans-2-Phenylcyclopropyl isocyanate 35661-60-0 35856-62-3, Piperidinesulfonyl chloride 36768-62-4, 4-Amino-2,2,6,6-tetramethylpiperidine 37736-82-6 37784-17-1 38212-30-5, 1 4-Methoxyphenyl piperazine 40203-94-9 41195-90-8, 2,3-Dichlorophenyl isocyanate 41483-72-1 42389-62-8 42406-72-4 46741-65-5 47375-34-8 50541-93-0, 4-Amino-1-benzylpiperidine 51207-66-0

Searched by P. Ruppel

51387-90-7, 2 2 Aminoethyl 1 methylpyrrolidine 51388-02-4 52616-82-7
54132-75-1, 3,5-Dimethylphenyl isocyanate 54997-90-9 55456-41-2
57177-83-0 59025-55-7, 2,4-Difluorophenyl isocyanate 59377-19-4,
4-Phenoxyphenyl isocyanate 59480-92-1, 2,5-Dimethyl-3-pyrroline
61342-80-1 62129-39-9 62368-55-2 63448-63-5, 2-Amino-1-methoxybutane
64030-44-0 66713-87-9 71989-40-7 73713-79-8, Benzo-2,1,3-thiadiazole-
4-sulfonyl chloride 79286-79-6, 3-Aminopyrrolidine 79777-82-5
80466-79-1, 3,5-Dimethylisoxazole-4-sulfonyl chloride 87206-44-8,
D-Methioninol 88398-93-0, 5-Chloro-1,3-dimethylpyrazole-4-sulfonyl
chloride 89007-45-4, 4-Isopropylphenyl isothiocyanate 93138-61-5,
3-(Aminomethyl)-1-benzylpyrrolidine 101364-00-5 104504-43-0
109523-13-9 114636-31-6 114715-38-7 114715-39-8 118684-31-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of peptidyl calcium channel blockers)

IT 123536-15-2 125741-65-3 443692-93-1, 7-Quinolinesulfonyl chloride
443692-98-6 443692-99-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of peptidyl calcium channel blockers)

IT 2130-96-3DP, resin-bound 16652-64-5DP, resin-bound 27817-35-2P
133852-23-0P 141595-75-7P 141595-76-8P 189264-75-3P 195708-10-2P
195708-11-3P 217172-22-0P 217172-23-1P 217172-30-0P 217172-31-1P
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248923-03-7P 248923-04-8P 248923-05-9P 248923-08-2P 443692-60-2P
443692-61-3P 443692-62-4P 443692-64-6P 443692-65-7P 443692-66-8P
443692-67-9P 443692-68-0P 443692-69-1P 443692-70-4P 443692-71-5P
443692-72-6P 443692-73-7P 443692-74-8P 443692-75-9P 443692-76-0P
443692-77-1P 443692-78-2P 443692-79-3DP, resin-bound 443692-80-6P
443692-81-7P 443692-82-8P 443692-83-9P 443692-84-0P 443692-85-1P
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443693-13-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation of peptidyl calcium channel blockers)

RE.CNT 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

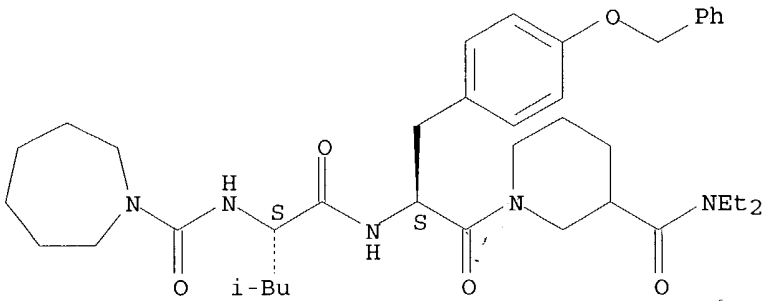
(1) Anon; EP 0482539 A2 1992 HCAPLUS
(2) Anon; WO 9306127 1993 HCAPLUS
(3) Anon; WO 9512612 1995 HCAPLUS
(4) Anon; WO 9620725 1996 HCAPLUS
(5) Anon; WO 9622966 1996 HCAPLUS
(6) Ishikawa; US 5496928 A 1996 HCAPLUS
(7) Ruger; US 5116835 A 1992 HCAPLUS

IT **443691-76-7P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)
(preparation of peptidyl calcium channel blockers)

RN 443691-76-7 HCAPLUS

CN 1H-Azepine-1-carboxamide, N-[(1S)-1-[[[(1S)-2-[3-[(diethylamino)carbonyl]-
1-piperidinyl]-2-oxo-1-[[4-(phenylmethoxy)phenyl]methyl]ethyl]amino]carbon
yl]-3-methylbutyl]hexahydro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L42 ANSWER 5 OF 101 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1999:344836 HCAPLUS
DN 131:689
ED Entered STN: 07 Jun 1999
TI Small molecule intervention in HIV-1 replication
IN Czarnik, Anthony William; Mack, David Phillip; Mei, Houng-Yau; Moreland, David Winslow
PA Warner-Lambert Company, USA
SO PCT Int. Appl., 46 pp.
CODEN: PIXXD2
DT **Patent**
LA English
IC ICM A61K031-00
CC 1-5 (Pharmacology)
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 9925327	A2	19990527	WO 1998-US19358	19980916 <--
WO 9925327	A3	19990923		

W: AL, AU, BA, BB, BG, BR, CA, CN, CU, CZ, EE, GE, HR, HU, ID, IL, IS, JP, KP, KR, LC, LK, LR, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, SL, TR, TT, UA, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

AU 9893182	A1	19990607	AU 1998-93182	19980916 <--
PRAI US 1997-65559P	P	19971114 <--		
WO 1998-US19358	W	19980916		

OS MARPAT 131:689
AB A series of small mols. which are inhibitors of HIV-1 Tat-TAR interaction is disclosed. The compds. are useful in the treatment of HIV-1 infections. Compds. of the invention include quinoxalinediones and diaminoquinazolines.
ST HIV1 Tat TAR interaction inhibitor; quinoxalinedione HIV1 Tat TAR interaction inhibitor; diaminoquinazoline HIV1 Tat TAR interaction inhibitor
IT Genetic element
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(TAR element; small mol. intervention in HIV-1 replication)
IT Structure-activity relationship
(Tat-TAR inhibiting; small mol. intervention in HIV-1 replication)
IT Transcriptional regulation
(activation; small mol. intervention in HIV-1 replication)

IT Structure-activity relationship
(antiviral; small mol. intervention in HIV-1 replication)
IT Antiviral agents
Human immunodeficiency virus 1
(small mol. intervention in HIV-1 replication)
IT Transcription factors
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(tat; small mol. intervention in HIV-1 replication)
IT 161516-37-6
RL: BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); PROC (Process)
(TAR31; small mol. intervention in HIV-1 replication)
IT 207004-60-2
RL: BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); PROC (Process)
(Tat40, Tat amino-terminal fragment; small mol. intervention in HIV-1 replication)
IT 201-09-2, Indeno[7,1-fg]quinoxaline 607-28-3 1899-48-5D,
2,4-Quinazolinediamine, derivs. 2213-63-0 2379-56-8 2379-57-9
13741-90-7, 2,4,6-Quinazolinetriamine 13794-43-9 14003-34-0
15804-19-0 15804-19-0D, derivs. 18671-95-9 20198-19-0 22310-38-9
25983-13-5 37764-41-3 53745-23-6 61875-42-1 72628-76-3
76097-87-5 78115-66-9 118876-57-6 118876-58-7 118876-78-1
118876-88-3 143948-51-0 156694-08-5 156694-76-7 156694-78-9
156695-02-2 171619-98-0 171620-01-2 179265-27-1 179265-34-0
179265-41-9 179265-43-1 179265-44-2 179265-45-3 179265-48-6
179265-50-0 179265-51-1 179265-54-4 179265-55-5 179265-59-9
179265-61-3 179265-63-5 179265-65-7 183545-80-4 183545-87-1
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202981-90-6 215182-73-3 215182-74-4, 2,4,5,6-Quinazolinetetramine
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225504-37-0 225504-38-1 225504-39-2 225504-40-5 225504-41-6
225504-42-7 225504-43-8 225504-44-9 225504-45-0 225504-46-1
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225504-72-3 **225504-73-4** 225504-74-5 225504-75-6
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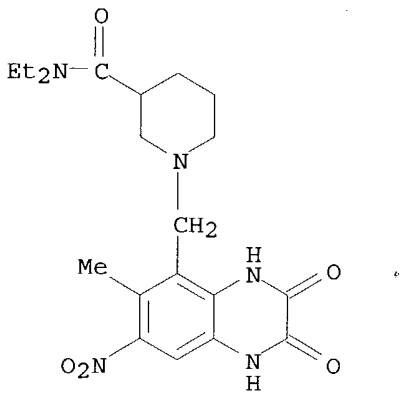
225504-81-4 225504-82-5 225504-83-6 225504-84-7 225504-85-8
225504-86-9 225504-87-0 225504-88-1 225504-89-2 225504-90-5
225504-91-6 225514-91-0 225514-92-1
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(small mol. intervention in HIV-1 replication)
IT **225504-73-4**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(small mol. intervention in HIV-1 replication)

RN 225504-73-4 HCAPLUS
CN 3-Piperidinecarboxamide, N,N-diethyl-1-[(1,2,3,4-tetrahydro-6-methyl-7-nitro-2,3-dioxo-5-quinoxalinyl)methyl]- (9CI) (CA INDEX NAME)



L42 ANSWER 10 OF 101 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1998:146699 HCAPLUS
DN 128:205145
ED Entered STN: 11 Mar 1998
TI Piperidine, pyrrolidine and hexahydro-1H-azepine peptide analogs promote release of growth hormone
IN Chen, Meng H.; Nargund, Ravi; Patchett, Arthur A.; Yang, Lihu
PA Merck and Co., Inc., USA
SO U.S., 95 pp., Cont.-in-part of U.S. 5,492,920.
CODEN: USXXAM
DT **Patent**
LA English
IC ICM A61K031-445
ICS C07D401-02; C07D401-14; C07D409-02
NCL 514318000
CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 2, 18, 63
FAN.CNT 6

	PATENT NO.	KIND	DATE		APPLICATION NO.	DATE	
PI	US 5721251	A	19980224		US 1996-600912	19960213	<--
	US 5492920	A	19960220		US 1994-323998	19941017	<--
PRAI	US 1993-165149		19931210	<--			
	US 1994-323998		19941017	<--			

OS MARPAT 128:205145
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The present invention = directed to certain novel compds. identified as substituted piperidines, pyrrolidines and hexahydro-1H-azepines of the general structural formula I [R1 = e.g., C1-10 alkyl, aryl, aryl(C1-6 alkyl); R3 = e.g., (CH2)q-Ph, (CH2)q-naphthyl, C3-7 cycloalkyl; X = e.g., H, cyano; Y = e.g., H, C1-10 alkyl; R4 and R5 = independently, e.g., H, C1-6 alkyl; A = (CH2)xCR7R7a(CH2)y, Z(CH2)xCR7R7a(CH2)y; x, y = 0-3; Z =

NR6a, O; R6a = H, C1-6 alkyl; R7, R7a = independently, e.g., H, C1-6 alkyl, CF3; n = 1-3; q = 0-3]. These compds. promote the release of growth hormone in humans and animals (no data). This property can be utilized to promote the growth of food animals to render the production of edible meat products more efficient, and in humans, to treat physiol. or medical conditions characterized by a deficiency in growth hormone secretion, such as short stature in growth hormone deficient children, and to treat medical conditions which are improved by the anabolic effects of growth hormone. Growth hormone releasing compns. containing such compds. as the active ingredient thereof are also disclosed. Thus, e.g., amide coupling of phenylpiperidine II.HCl (preparation given) with (2R)-N-Boc-amino-5-phenylpentanoic acid followed by deprotection and coupling with N-Boc-α-methylalanine and deprotection afforded piperidine derivative III.HCl.

ST growth hormone release factor peptide analog; piperidine peptide growth hormone release stimulant; pyrrolidine peptide growth hormone release stimulant; azepine hexahydro growth hormone release stimulant

IT 170840-09-2P 170840-15-0P 176705-91-2P 176705-92-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); FFD (Food or feed use); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of piperidine, pyrrolidine, and hexahydroazepine peptide analogs as growth hormone release promoters)

IT

170837-86-2P	170838-32-1P	170838-33-2P	170840-07-0P	170840-08-1P
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203941-77-9P 203941-99-5P 203942-00-1P 203942-01-2P
203942-02-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); FFD (Food or feed use); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of piperidine, pyrrolidine, and hexahydroazepine peptide analogs as growth hormone release promoters)

IT 203942-03-4P 203942-04-5P 203942-05-6P 203942-06-7P 203942-07-8P
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203942-31-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); FFD (Food or feed use); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of piperidine, pyrrolidine, and hexahydroazepine peptide analogs as growth hormone release promoters)

IT 9002-72-6, Growth hormone
RL: BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study)
(preparation of piperidine, pyrrolidine, and hexahydroazepine peptide analogs as growth hormone release promoters)

IT 176705-72-9P 176705-73-0P
RL: PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of piperidine, pyrrolidine, and hexahydroazepine peptide analogs as growth hormone release promoters)

IT 96-26-4, 1,3-Dihydroxyacetone 98-10-2, Benzenesulfonamide 98-80-6, Phenylboronic acid 100-51-6, Benzenemethanol, reactions 107-18-6, 2-Propen-1-ol, reactions 110-86-1, Pyridine, reactions 110-87-2, Dihydropyran 110-91-8, Morpholine, reactions 123-75-1, Pyrrolidine, reactions 501-53-1, Benzyl chloroformate 504-63-2, 1,3-Propanediol 541-41-3, Ethyl chloroformate 614-18-6, Ethyl nicotinate 623-33-6, Glycine ethyl ester hydrochloride 867-13-0, Triethyl phosphonoacetate 934-56-5, Trimethylphenyltin 1074-16-4, 2-Bromophenethyl alcohol 1820-80-0, 5-Aminopyrazole 1943-83-5, 2-Chloroethyl isocyanate 2279-15-4, N-Cbz-D-tryptophan 2304-94-1 2537-48-6, Diethyl (cyanomethyl)phosphonate 2627-86-3, (S)-α-Methylbenzylamine 3886-69-9, (R)-α-Methylbenzylamine 4644-61-5, 3-Ethoxycarbonyl-4-piperidone hydrochloride 5241-64-5 5271-38-5, 2-(Methylthio)ethanol 6630-33-7, 2-Bromobenzaldehyde 7764-95-6, Boc-D-alanine 13325-10-5, 4-Aminobutanol 14222-20-9 15030-72-5, N-Cbz-α-methylalanine 17392-83-5 18542-42-2, 2-(Methylthio)ethylamine 18982-54-2, 2-Bromobenzyl alcohol 21299-81-0 24424-99-5, Di-tert-butyl dicarbonate 30992-29-1, N-Boc-α-methylalanine 31602-63-8, 5-(Aminomethyl)tetrazole 33458-51-4 41253-21-8, Sodium 1,2,4-triazole

47173-80-8 54755-77-0 71486-53-8 84358-13-4, N-tert-Butoxycarbonylisonipecotic acid 120570-05-0, (S)-3-Aminoquinuclidine 129765-95-3 156130-68-6 163438-09-3, (R)-N-tert-Butoxycarbonylnipecotic acid 197900-84-8 203869-80-1 203869-85-6 203941-83-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of piperidine, pyrrolidine, and hexahydroazepine peptide analogs as growth hormone release promoters)

IT 17100-66-2P 25162-45-2P 25162-46-3P 57092-18-9P 115509-01-8P
121148-97-8P 124508-74-3P 126090-33-3P 141595-98-4P 148471-65-2P
159634-88-5P 159634-89-6P 159634-93-2P 159634-94-3P 159635-47-9P
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170837-75-9P 170837-76-0P 170837-78-2P 170837-81-7P 170837-83-9P
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170837-90-8P 170837-92-0P 170837-93-1P 170837-94-2P 170837-95-3P
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170838-22-9P 170838-23-0P 170838-25-2P 170838-28-5P 170838-34-3P
170838-35-4P 170838-36-5P 170838-37-6P 170838-39-8P 170838-40-1P
170838-41-2P 170838-42-3P 170838-44-5P 170838-45-6P 170838-47-8P
170838-48-9P 170838-49-0P 170838-52-5P 170838-54-7P 170838-55-8P
170838-56-9P 170838-60-5P 170838-61-6P 170838-62-7P 170838-63-8P
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197900-38-2P 197900-39-3P 197900-42-8P 197900-77-9P 197900-78-0P
197900-85-9P 198083-88-4P 198083-89-5P 198083-90-8P 198083-91-9P
198083-92-0P 198083-94-2P 198083-95-3P 203869-49-2P 203941-20-2P
203941-21-3P 203941-78-0P 203941-79-1P 203941-80-4P 203941-81-5P
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203941-93-9P 203941-94-0P 203941-95-1P 203941-96-2P 203941-97-3P
203941-98-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of piperidine, pyrrolidine, and hexahydroazepine peptide analogs as growth hormone release promoters)

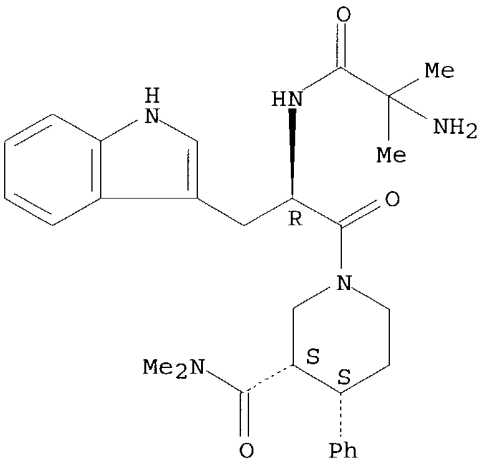
RE.CNT 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Ammann; Am J Physiology 1993, V265, PE770 HCAPLUS
(2) Anon; EP 0144230 A3 1985 HCAPLUS
(3) Anon; JP 05-163224 1993 HCAPLUS
(4) Anon; WO 9407486 1994 HCAPLUS
(5) Anon; WO 9408583 1994 HCAPLUS
(6) Anon; WO 9413696 1994 HCAPLUS
(7) Anon; WO 9419367 1994 HCAPLUS
(8) Anon; WO 9513069 1995 HCAPLUS
(9) Asato; US 4036979 1977 HCAPLUS
(10) Bochis; US 5283241 1994 HCAPLUS
(11) Chen; US 5492920 1996 HCAPLUS
(12) Chu; US 5284841 1994 HCAPLUS

(13) Dimarchi; US 4782139 1988 HCAPLUS
(14) Fisher; US 5206235 1993 HCAPLUS
(15) Fisher; US 5310737 1994 HCAPLUS
(16) Fisher; US 5606054 1997 HCAPLUS
(17) Hodge; US 3239345 1966 HCAPLUS
(18) Horwell; 1990 HCAPLUS
(19) Momany; US 4411890 1983 HCAPLUS
(20) Morriello; US 5492916 1996 HCAPLUS
(21) Morriello; US 5494919 1996 HCAPLUS
(22) Ok; US 5317017 1994 HCAPLUS
(23) Recker; US 5164368 1992 HCAPLUS
(24) Sakamoto; 1990 HCAPLUS
(25) Seely; US 5137872 1992 HCAPLUS
(26) Smith, R; Science, Reprint Series 1993, V260, P1640 HCAPLUS
(27) Tuggle; US 5614364 1997 HCAPLUS

IT **170840-68-3P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); FFD (Food or feed use); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of piperidine, pyrrolidine, and hexahydroazepine peptide analogs as growth hormone release promoters)

RN 170840-68-3 HCAPLUS
CN 3-Piperidinecarboxamide, N,N-dimethyl-1-[N-(2-methylalanyl)-D-tryptophyl]-4-phenyl-, monohydrochloride, (3S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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L42 ANSWER 15 OF 101 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1997:471325 HCAPLUS
DN 127:161690
ED Entered STN: 26 Jul 1997
TI Preparation of 2,5-diaryltetrahydrofurans for the treatment of inflammatory and immune disorders
IN Cai, Xiong; Hussoin, Sajjat; Hwang, San-Bao; Killian, David; Shen, T. Y.
PA Cytomed, Inc., USA

SO U.S., 27 pp., Cont.-in-part of U.S. 5,434,151.
CODEN: USXXAM
DT **Patent**
LA English
IC ICM C07D333-22
ICS C07D413-00
NCL 544124000
CC 27-6 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1
FAN.CNT 5

	PATENT NO.	KIND	DATE		APPLICATION NO.	DATE	
PI	US 5648486	A	19970715		US 1993-62391	19930512	<--
	US 5358938	A	19941025		US 1992-912788	19920713	<--
	US 5434151	A	19950718		US 1992-933991	19920824	<--
	WO 9401430	A1	19940120		WO 1993-US6575	19930713	<--
	W: AU, CA, FI, HU, JP, KR						
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE						
	AU 9347722	A1	19940131		AU 1993-47722	19930713	<--
	AU 666578	B2	19960215				
	EP 650485	A1	19950503		EP 1993-918182	19930713	<--
	EP 650485	B1	20001011				
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE						
	HU 72601	A2	19960528		HU 1995-99	19930713	<--
	AT 196903	E	20001015		AT 1993-918182	19930713	<--
	ES 2152952	T3	20010216		ES 1993-918182	19930713	<--
	PT 650485	T	20010330		PT 1993-918182	19930713	<--
	US 5463083	A	19951031		US 1994-178222	19940106	<--
	US 5741809	A	19980421		US 1995-466332	19950606	<--
	US 6294574	B1	20010925		US 1995-469073	19950606	<--
	US 5856323	A	19990105		US 1995-481812	19950607	<--
	US 2002177723	A1	20021128		US 2000-547941	20000411	<--
	GR 3035063	T3	20010330		GR 2000-402751	20001213	<--
PRAI	US 1992-912788	A3	19920713	<--			
	US 1992-933991	A2	19920824	<--			
	US 1992-933911	A2	19920824	<--			
	US 1993-62391	A	19930512	<--			
	WO 1993-US6575	A	19930713	<--			
	US 1994-178222	A3	19940106	<--			
	US 1995-469073	A1	19950606	<--			

OS MARPAT 127:161690
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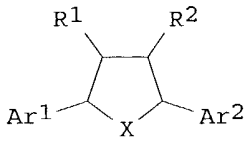

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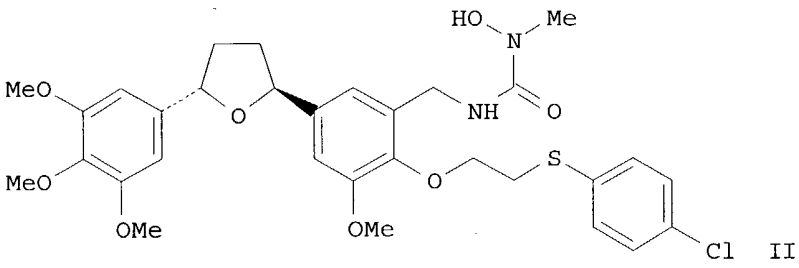

II

AB The title compds. [I; Ar1, Ar2 = substituted aryl, pyridyl; X = O, S, S(O), S(O)2, CR9NR10; R1, R2 = H, halo, lower alkyl, etc.; R9 = H, halo, lower alkyl, etc.; R10 = cyclic and acyclic alkyl, alkenyl, etc.] that reduce the chemotaxis and respiratory burst leading to the formation of damaging oxygen radicals of polymorphonuclear leukocytes during an inflammatory or immune response, were prepared The compds. I exhibit this biol. activity by acting as PAF receptor antagonists, by inhibiting the enzyme 5-lipoxygenase, or by exhibiting dual activity, i.e., by acting as both a PAF receptor antagonist and inhibitor of 5-lipoxygenase. Thus, 11-step synthesis of the title compound trans-II which showed IC50 of 7.60 nM against PAF and of 22.2 nM against 5-LO, is described.

ST aryltetrahydrofuran prepn inflammatory immunol disorder; antiinflammatory aryltetrahydrofuran prepn; PAF receptors antagonist aryltetrahydrofuran prepn; platelet activating factor receptor aryltetrahydrofuran prepn; lipoxygenase inhibitor aryltetrahydrofuran prepn

IT Platelet-activating factor receptors
RL: BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study)
(PAF receptors antagonists; preparation of 2,5-diaryltetrahydrofurans for the treatment of inflammatory and immune disorders)

IT Immunity
(disorder, treatment of; preparation of 2,5-diaryltetrahydrofurans for the treatment of inflammatory and immune disorders)

IT Anti-inflammatory agents
(preparation of 2,5-diaryltetrahydrofurans for the treatment of inflammatory and immune disorders)

IT 80619-02-9, 5-Lipoxygenase
RL: BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study)
(inhibitors; preparation of 2,5-diaryltetrahydrofurans for the treatment of inflammatory and immune disorders)

IT 193738-95-3P 193738-96-4P 193738-97-5P 193738-98-6P 193738-99-7P
193739-00-3P 193739-01-4P 193739-02-5P 193739-03-6P 193739-04-7P
193739-05-8P 193739-06-9P 193739-07-0P 193739-08-1P 193739-09-2P
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193739-15-0P **193739-16-1P** 193739-17-2P **193739-18-3P**
193739-19-4P 193739-20-7P 193739-22-9P 193739-23-0P 193739-24-1P
193739-25-2P 193739-26-3P 193739-27-4P 193739-28-5P 193739-29-6P

193739-30-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 2,5-diaryltetrahydrofurans for the treatment of inflammatory and immune disorders)

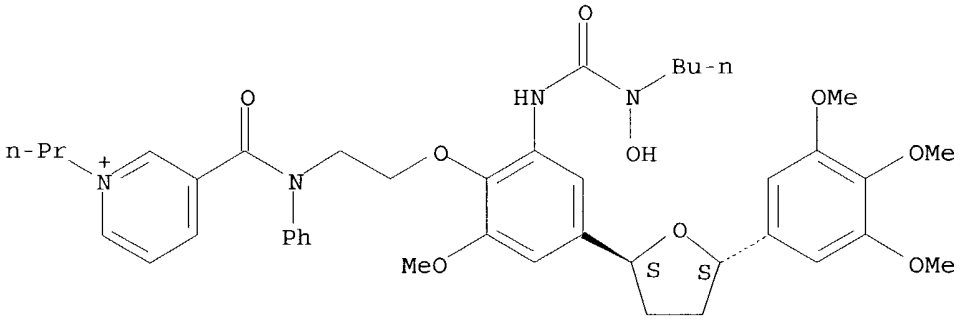
IT 106-54-7, 4-Chlorothiophenol 1136-86-3 5438-36-8, 5-Iodovanillin
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of 2,5-diaryltetrahydrofurans for the treatment of inflammatory and immune disorders)

IT 39038-42-1P 106331-50-4P 134169-61-2P 154544-29-3P 154544-30-6P 154544-31-7P 171095-72-0P 171095-73-1P 193739-31-0P 193739-32-1P 193739-33-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 2,5-diaryltetrahydrofurans for the treatment of inflammatory and immune disorders)

IT **193739-16-1P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 2,5-diaryltetrahydrofurans for the treatment of inflammatory and immune disorders)

RN 193739-16-1 HCAPLUS
CN Pyridinium, 3-[[[2-[2-[[(butylhydroxyamino)carbonyl]amino]-6-methoxy-4-[tetrahydro-5-(3,4,5-trimethoxyphenyl)-2-furanyl]phenoxy]ethyl]phenylamino]carbonyl]-1-propyl-, iodide, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



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L42 ANSWER 20 OF 101 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1996:756604 HCAPLUS
DN 126:14765
ED Entered STN: 26 Dec 1996
TI Agent for the treatment of severe acute pancreatitis
IN Inatomi, Nobuhiro; Takatani, Muneo
PA Takeda Chemical Industries, Ltd., Japan; Inatomi, Nobuhiro; Takatani, Muneo
SO PCT Int. Appl., 55 pp.
CODEN: PIXXD2
DT **Patent**

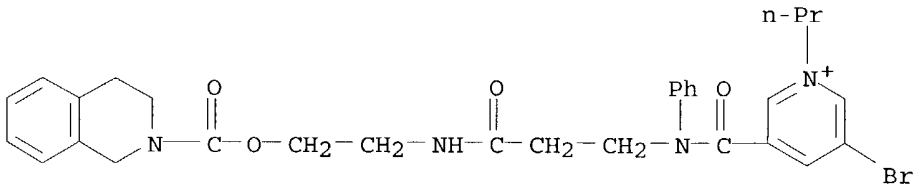
LA English
IC ICM A61K031-47
CC 1-9 (Pharmacology)
Section cross-reference(s): 63
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9633718	A1	19961031	WO 1996-JP1138	19960425 <--
	W: AL, AM, AU, AZ, BB, BG, BR, BY, CA, CN, CZ, EE, GE, HU, IS, KG, KR, KZ, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TR, TT, UA, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU				
	RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	AU 9655141	A1	19961118	AU 1996-55141	19960425 <--
	JP 09151133	A2	19970610	JP 1996-105937	19960426 <--
PRAI	JP 1995-104247		19950427 <--		
	JP 1995-245657		19950925 <--		
	WO 1996-JP1138		19960425 <--		

OS MARPAT 126:14765
AB This invention provides a prophylactic and/or therapeutic agent for severe acute pancreatitis which comprises a pyridinium compound, preferably 3-bromo-5-[N-phenyl-N-[2-[[-(1,2,3,4-tetrahydro-2-isoquinolylcarbonyloxy)ethyl]carbamoyl]ethyl]carbamoyl]-1-propylpyridinium nitrate (I). I was tested for its effect on aggravation by endotoxemia in rats with taurocholate-induced pancreatitis; I suppressed increased lethality, ascites fluid leakage, coagulation disorders, and renal dysfunctions in acute pancreatitis. An injection solution containing I 10 mg/mL was formulated.
ST acute pancreatitis pyridinium isoquinolyl deriv injection
IT Pancreas, disease
(acute necrotizing pancreatitis; pyridinium compds. for treatment of severe acute pancreatitis)
IT Pancreas, disease
(acute pancreatitis; pyridinium compds. for treatment of severe acute pancreatitis)
IT Pancreas, disease
(acute, hemorrhagic; pyridinium compds. for treatment of severe acute pancreatitis)
IT Drug delivery systems
(injections; pyridinium compds. for treatment of severe acute pancreatitis)
IT **131311-25-6**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(pyridinium compds. for treatment of severe acute pancreatitis)
IT **131311-25-6**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(pyridinium compds. for treatment of severe acute pancreatitis)
RN 131311-25-6 HCAPLUS
CN Pyridinium, 3-bromo-5-[[[3-[[2-[[(3,4-dihydro-2(1H)-isoquinolinyl)carbonyl]oxy]ethyl]amino]-3-oxopropyl]phenylamino]carbonyl]-1-propyl-, nitrate (9CI) (CA INDEX NAME)

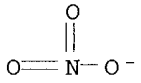
CM 1

CRN 131311-24-5
CMF C30 H34 Br N4 O4



CM 2

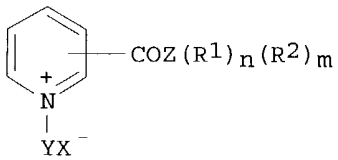
CRN 14797-55-8
CMF N O3



L42 ANSWER 25 OF 101 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1996:377493 HCAPLUS
DN 125:117302
ED Entered STN: 29 Jun 1996
TI Fabric conditioners and softening agents derived from pyridiniumcarboxylate esters or pyridiniumcarboxamides
IN Wu, Shang Ren; Gutierrez, Eddie N.
PA Lever Brothers Company, Division of Conopco, Inc., USA
SO U.S., 4 pp., Cont.-in-part of U.S. 5,419,843.
CODEN: USXXAM
DT **Patent**
LA English
IC ICM D06M013-46
NCL 252008800
CC 40-7 (Textiles and Fibers)
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5520828	A	19960528	US 1995-380786	19950130 <--
	US 5419843	A	19950530	US 1994-262074	19940616 <--
PRAI	US 1994-262074		19940616 <--		

OS MARPAT 125:117302
GI



I

AB Novel biodegradable fabric conditioners based on pyridiniumcarboxylate esters or amides are of general formula I [COZ(R1)n(R2)m is a monosubstituted ester- or amide-linked moiety; Z = O, NH, or N; Y = C1-3-alkyl; X- is a water-soluble anion; R1,R2 = alkyl, alkenyl, alkoxy, or R1R2 = a C16-50-substituent; n = 0-1, m = 1.]. Preferred compns. include I (when Z = O or NH, R2 = C24-40-linear or branched alkyl; when Z = N, R1 and R2 are each C16-25-alkyl); X- is selected from Cl-, Br-, I-, and MeOSO3-.

ST biodegradable pyridiniumcarboxylate fabric softener conditioner; pyridiniumcarboxamide biodegradable fabric softener conditioner

IT Biodegradable materials
Softening agents
(fabric conditioners and softening agents derived from pyridiniumcarboxylate esters or pyridiniumcarboxamides)

IT Pyridinium compounds
RL: BPR (Biological process); BSU (Biological study, unclassified); NUU (Other use, unclassified); BIOL (Biological study); PROC (Process); USES (Uses)
(fabric conditioners and softening agents derived from pyridiniumcarboxylate esters or pyridiniumcarboxamides)

IT Textiles
(manufacture of; fabric conditioners and softening agents derived from pyridiniumcarboxylate esters or pyridiniumcarboxamides)

IT 34452-78-3D, C24-28-esters **168544-21-6**
RL: BPR (Biological process); BSU (Biological study, unclassified); NUU (Other use, unclassified); BIOL (Biological study); PROC (Process); USES (Uses)
(fabric conditioners and softening agents derived from pyridiniumcarboxylate esters or pyridiniumcarboxamides)

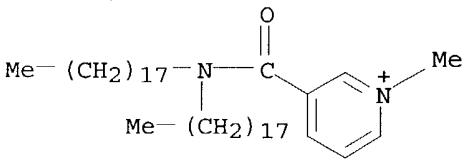
IT **168544-21-6**
RL: BPR (Biological process); BSU (Biological study, unclassified); NUU (Other use, unclassified); BIOL (Biological study); PROC (Process); USES (Uses)
(fabric conditioners and softening agents derived from pyridiniumcarboxylate esters or pyridiniumcarboxamides)

RN 168544-21-6 HCAPLUS

CN Pyridinium, 3-[(dioctadecylamino)carbonyl]-1-methyl-, methyl sulfate (9CI) (CA INDEX NAME)

CM 1

CRN 168544-20-5
CMF C43 H81 N2 O



CM 2

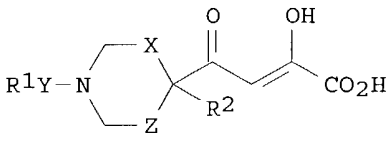
CRN 21228-90-0
CMF C H3 O4 S

Me—O—SO_3^-

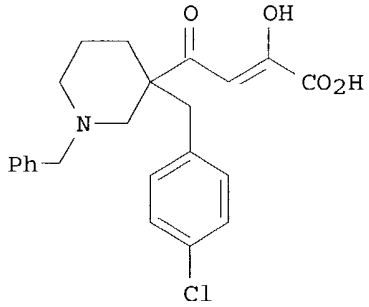
L42 ANSWER 30 OF 101 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1996:35029 HCAPLUS
DN 124:232250
ED Entered STN: 18 Jan 1996
TI Piperidinyldioxobutanoic acid derivatives as inhibitors of influenza endonuclease
IN Selnick, Harold G.; Ponticello, Gerald S.; Baldwin, John J.; Tomassini, Joanne E.
PA Merck and Co., Inc., USA
SO U.S., 16 pp.
CODEN: USXXAM
DT **Patent**
LA English
IC ICM C07D211-32
ICS C07D401-06
NCL 546225000
CC 27-16 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1, 63
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5475109	A	19951212	US 1994-324190	19941017 <--
	US 5618830	A	19970408	US 1995-536294	19950929 <--
	GB 2294264	A1	19960424	GB 1995-20625	19951009 <--
	GB 2294264	B2	19981014		
PRAI	US 1994-324190		19941017 <--		

OS MARPAT 124:232250
GI



I



II

AB Dioxobutanoic acids substituted with piperidine or similar N-substituted saturated cycloalkyls, I or pharmaceutically acceptable salt, hydrate or crystal forms thereof, wherein: X is CH2, CH2CH2, or a bond; Z is CH2, CH2CH2, or a bond; Y is CH2 , CO, SO2, or a bond; R1 and R2 are independently selected from the following: branched or unbranched C1-6 alkyl, C1-6 alkyloxy, NC1-6 alkyl, C3-8 cycloalkyl, Ph, naphthyl, pyridyl, furanyl, thienyl, or quinolinyl, any of which may be substituted once or twice with C1-5 alkyl, C3-8 cycloalkyl, Ph, quinolinyl, pyridyl, furanyl, thienyl, C1-6-alkoxy, Br, F, or Cl, are found to inhibit the cap-dependent endonuclease of influenza virus. These compds. are useful in the prevention or treatment of infection by influenza virus and the treatment of influenza, either as compound, pharmaceutically acceptable salts, pharmaceutical composition ingredients, whether or not in combination with other antivirals, immunomodulators, antibiotics or vaccines. Methods of treating influenza and methods of preventing or treating infection by influenza virus are also described. Thus, e.g., treatment of N-benzyl-3-acetyl-3-(4-chlorobenzyl)piperidine with di-Me oxalate and NaH followed by HCl afforded 4-[N-benzyl-3-(4-chlorobenzyl)-piperidin-3-yl]-2,4-dioxobutanoic acid hydrochloride (II.HCl) which inhibited alfalfa mosaic virus primed flu transcription with IC50 = 1.1 μM.

ST influenza endonuclease inhibitor piperidinyldioxobutanoic acid deriv

IT Influenza
(A, piperidinyldioxobutanoic acid derivs. as inhibitors of influenza endonuclease)

IT Influenza
(B, piperidinyldioxobutanoic acid derivs. as inhibitors of influenza endonuclease)

IT 9055-11-2, Endonuclease
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(influenza; piperidinyldioxobutanoic acid derivs. as inhibitors of influenza endonuclease)

IT 160428-89-7P 174605-58-4P 174605-59-5P 174605-60-8P 174605-61-9P
174605-62-0P 174605-63-1P 174605-64-2P 174605-65-3P 174605-66-4P
174605-67-5P 174605-68-6P 174605-69-7P 174605-70-0P 174605-71-1P
174605-72-2P 174605-73-3P 174605-74-4P 174605-75-5P 174605-76-6P
174605-77-7P 174605-78-8P 174605-79-9P 174605-80-2P 174605-81-3P
174605-82-4P 174605-83-5P 174605-84-6P 174605-85-7P 174605-86-8P
174605-87-9P 174605-88-0P 174605-89-1P 174605-90-4P 174605-92-6P
174605-93-7P 174605-94-8P 174605-95-9P 174605-96-0P 174605-97-1P
174605-98-2P 174605-99-3P 174606-00-9P 174606-01-0P 174606-02-1P
174606-03-2P 174606-04-3P 174606-05-4P 174606-06-5P 174606-07-6P
174606-08-7P 174606-09-8P 174606-10-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(piperidinyldioxobutanoic acid derivs. as inhibitors of influenza endonuclease)

IT 98-09-9, Benzenesulfonyl chloride 100-44-7, Benzyl chloride, reactions
104-83-6, 4-Chlorobenzyl chloride 1126-09-6, Ethyl isonipecotate
130250-54-3, Ethyl N-Boc-nipecotate 142851-03-4, Ethyl N-Boc-isonipecotate
RL: RCT (Reactant); RACT (Reactant or reagent)
(piperidinyldioxobutanoic acid derivs. as inhibitors of influenza endonuclease)

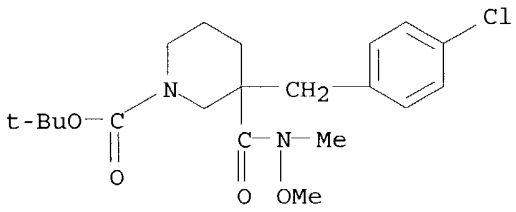
IT 111627-26-0P 170284-71-6P 174605-91-5P 174606-11-2P 174606-12-3P
174606-13-4P 174606-14-5P 174606-15-6P 174606-16-7P
174606-17-8P 174606-18-9P 174606-19-0P 174606-20-3P
174606-21-4P 174606-22-5P 174606-23-6P 174606-24-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(piperidinyldioxobutanoic acid derivs. as inhibitors of influenza endonuclease)

IT **174606-17-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(piperidinyldioxobutanoic acid derivs. as inhibitors of influenza endonuclease)

RN 174606-17-8 HCAPLUS

CN 1-Piperidinecarboxylic acid, 3-[(4-chlorophenyl)methyl]-3-[(methoxymethylamino)carbonyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



L42 ANSWER 35 OF 101 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1995:661074 HCAPLUS

DN 123:232063

ED Entered STN: 08 Jul 1995

TI Conditioning fabrics with biodegradable conditioners derived from pyridinecarboxylic acids

IN Wu, Shang Ren; Gutierrez, Eddie N.

PA Lever Brothers Co., USA

SO U.S., 4 pp.
CODEN: USXXAM

DT **Patent**

LA English

IC ICM D06M013-322
ICS D06M013-46

NCL 252088000

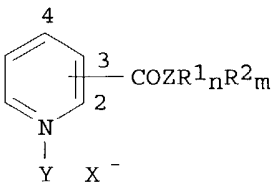
CC 46-5 (Surface Active Agents and Detergents)
Section cross-reference(s): 40

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5419843	A	19950530	US 1994-262074	19940616 <--
	US 5520828	A	19960528	US 1995-380786	19950130 <--
PRAI	US 1994-262074		19940616 <--		

OS MARPAT 123:232063

GI



I

AB Title method comprises contacting the fabric with a composition containing 1-99 weight% I (COZR1nR2m is a monosubstituted ester or its amide linked moiety which may be at the 2, 3, or 4 position on the pyridine ring; Y is a C1-3 alkyl; X is a water-soluble anion; R1, R2 is straight or branched alkyl, alkenyl, or alkoxy; R1 and R2 together have a total of 16-50 C; n is 0, 1; with the proviso that when Z is O or NH, n is 1, and R2 is a straight or branched C16-50 alkyl, alkenyl, or alkoxy; when Z is N, n is 1 and R1 and R2 are each straight or branched alkyl, alkenyl, or alkoxy and R1 and R2 together have a total of 16-50 C) and 99-1 weight% water to condition the fabric during a laundering process. The compds. are effective fabric conditioners and are biodegradable. I (R1, R2 = octadecyl; Z = O; n =1; Y = Me; X = methosulfate; 3-position) was prepared and used in a detergent composition to soften terry towels.

ST pyridiniumcarboxamide softener fabrics biodegradable; laundry detergent pyridiniumcarboxamide softener

IT Softening agents
(pyridiniumcarboxamide derivs. for fabrics)

IT Biodegradable materials
(pyridiniumcarboxamide derivs. softeners for fabrics)

IT Alcohols, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(C24-28, Guerbet, reaction products with nicotinic acid chloride; in manufacture of fabric-conditioning compound)

IT Detergents
(laundry, pyridiniumcarboxamide derivs. softeners for)

IT **168544-21-6P**
RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(fabric conditioning compound)

IT 168544-19-2P
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(in manufacture of fabric-conditioning compound)

IT 112-99-2, Dioctadecylamine 20260-53-1, Nicotinic acid chloride hydrochloride
RL: RCT (Reactant); RACT (Reactant or reagent)
(in manufacture of fabric-conditioning compound)

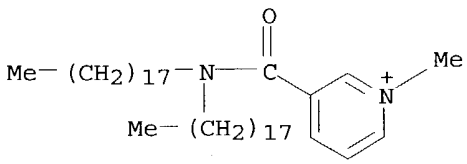
IT **168544-21-6P**
RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(fabric conditioning compound)

RN 168544-21-6 HCAPLUS

CN Pyridinium, 3-[(dioctadecylamino)carbonyl]-1-methyl-, methyl sulfate (9CI) (CA INDEX NAME)

CM 1

CRN 168544-20-5
CMF C43 H81 N2 O



CM 2

CRN 21228-90-0
CMF C H3 O4 S

Me—O—SO_3^-

L42 ANSWER 40 OF 101 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1994:153730 HCAPLUS
DN 120:153730
ED Entered STN: 02 Apr 1994
TI Synergistic combinations of PAF antagonists and anticholinergic agents as drugs for treatment of bronchial asthma.
IN Heuer, Hubert
PA Boehringer Ingelheim KG, Germany
SO Ger. Offen., 13 pp.
CODEN: GWXXBX
DT **Patent**
LA German
IC ICM A61K031-55
ICS A61K031-445
CC 1-9 (Pharmacology)
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI DE 4219659	A1	19931223	DE 1992-4219659	19920616 <--
PRAI DE 1992-4219659		19920616 <--		

OS MARPAT 120:153730
AB Mixts of hetrazepine derivative PAF antagonists (Markush given) with anticholinergics are synergistic drugs for treatment of bronchial asthma. The effectiveness of a combination of atropine with WEB 2170 was shown on PAF-induced bronchoconstriction, in guinea pigs.
ST synergism PAF antagonist anticholinergic bronchial asthma
IT Cholinergic antagonists
(drugs for treatment of bronchial asthma containing PAF antagonists and, synergistic)
IT Bronchodilators
(antiasthmatics, anticholinergic agent combinations with PAF antagonists, for treatment of bronchial asthma)
IT 153445-18-2
RL: BIOL (Biological study)
(drug for treatment of bronchial asthma, synergistic)
IT 50-10-2, Oxyphenonium bromide 51-56-9D, Homatropine hydrobromide, mixts. with hetrazepine derivative PAF antagonists 52-88-0D, Atropine methonitrate, mixts. with hetrazepine derivative PAF antagonists 53-46-3D, Methanthelinium bromide, mixts. with hetrazepine derivative PAF antagonists 54-30-8D, Camylofin, mixts. with hetrazepine derivative PAF antagonists 55-16-3D, Hyoscine hydrochloride, mixts. with hetrazepine derivative PAF antagonists 56-54-2D, Quinidine, mixts. with hetrazepine derivative PAF antagonists 58-34-4D, Thiazinamium methyl sulfate, mixts. with hetrazepine derivative PAF antagonists 59-92-7D, Levadopa, mixts. with hetrazepine derivative PAF antagonists 60-44-6D, Penthienate bromide, mixts. with hetrazepine derivative PAF antagonists 60-46-8D, Dimevamide, mixts. with hetrazepine derivative PAF antagonists 62-97-5D, Diphemanil, mixts. with hetrazepine derivative PAF antagonists 71-81-8D, Isopropamide iodide, mixts. with hetrazepine derivative PAF antagonists 76-90-4D, Mepenzolate bromide, mixts. with hetrazepine derivative PAF antagonists 77-19-0D, Dicycloverine, mixts.

with hetrazepine derivative PAF antagonists 77-37-2D, Procyclidine, mixts. with hetrazepine derivative PAF antagonists 77-39-4D, Cycrimine, mixts. with hetrazepine derivative PAF antagonists 80-49-9D, Homatropine methyl bromide, mixts. with hetrazepine derivative PAF antagonists 80-50-2D, Octatropine methyl bromide, mixts. with hetrazepine derivative PAF antagonists 82-98-4D, Piperidolate, mixts. with hetrazepine derivative PAF antagonists 82-99-5D, Tifenamil, mixts. with hetrazepine derivative PAF antagonists 86-24-8D, Antiparkin, mixts. with hetrazepine derivative PAF antagonists 90-22-2D, Barespan, mixts. with hetrazepine derivative PAF antagonists 90-23-3D, Piperphenidol, mixts. with hetrazepine derivative PAF antagonists 97-75-6D, Hyoscinamine oxide, mixts. with hetrazepine derivative PAF antagonists 100-91-4D, Eucatropine, mixts. with hetrazepine derivative PAF antagonists 101-31-5D, Hyoscyamine, mixts. with hetrazepine derivative PAF antagonists 115-51-5D, Ambutonium bromide, mixts. with hetrazepine derivative PAF antagonists 115-63-9D, Hexocyclium methyl sulfate, mixts. with hetrazepine derivative PAF antagonists 117-30-6D, Dipiproverine, mixts. with hetrazepine derivative PAF antagonists 125-51-9D, Pipenzolate bromide, mixts. with hetrazepine derivative PAF antagonists 125-53-1D, Oxyphencyclimine, mixts. with hetrazepine derivative PAF antagonists 125-85-9D, Caramiphenium chloride, mixts. with hetrazepine derivative PAF antagonists 132-17-2D, mixts. with hetrazepine derivative PAF antagonists 144-11-6D, Trihexyphenidyl, mixts. with hetrazepine derivative PAF antagonists 148-32-3D, Amprotropine, mixts. with hetrazepine derivative PAF antagonists 150-59-4D, Alverine, mixts. with hetrazepine derivative PAF antagonists 155-41-9D, Hyoscine methobromide, mixts. with hetrazepine derivative PAF antagonists 298-50-0D, Propantheline, mixts. with hetrazepine derivative PAF antagonists 302-40-9D, Benactyzine, mixts. with hetrazepine derivative PAF antagonists 312-45-8D, Hemicholinium bromide, mixts. with hetrazepine derivative PAF antagonists 428-07-9D, Atromepine, mixts. with hetrazepine derivative PAF antagonists 495-83-0D, Tigloidin, mixts. with hetrazepine derivative PAF antagonists 502-59-0D, Octamylamine, mixts. with hetrazepine derivative PAF antagonists 511-45-5D, Pridinol, mixts. with hetrazepine derivative PAF antagonists 511-55-7D, Xenytropium bromide, mixts. with hetrazepine derivative PAF antagonists 512-15-2D, Cyclopentolate, mixts. with hetrazepine derivative PAF antagonists 514-65-8D, Biperiden, mixts. with hetrazepine derivative PAF antagonists 520-20-7D, Mepiperphenidol, mixts. with hetrazepine derivative PAF antagonists 522-18-9D, Chlorbenzoxamine, mixts. with hetrazepine derivative PAF antagonists 524-83-4D, Etybenzatropine, mixts. with hetrazepine derivative PAF antagonists 532-49-0D, Dibuline sulfate, mixts. with hetrazepine derivative PAF antagonists 545-80-2D, Poldine methyl sulfate, mixts. with hetrazepine derivative PAF antagonists 561-43-3D, Oxypyrronium bromide, mixts. with hetrazepine derivative PAF antagonists 561-77-3D, Dihexyverine, mixts. with hetrazepine derivative PAF antagonists 561-79-5D, Metacaraphen, mixts. with hetrazepine derivative PAF antagonists 587-49-5D, Salfluverine, mixts. with hetrazepine derivative PAF antagonists 596-51-0D, Glycopyrronium bromide, mixts. with hetrazepine derivative PAF antagonists 604-51-3D, Deptropine, mixts. with hetrazepine derivative PAF antagonists 968-63-8D, Butinoline, mixts. with hetrazepine derivative PAF antagonists 1050-48-2D, Benzilonium bromide, mixts. with hetrazepine derivative PAF antagonists 1156-05-4D, Phenglutarimide, mixts. with hetrazepine derivative PAF antagonists 1164-38-1D, Lachesine, mixts. with hetrazepine derivative PAF antagonists 1232-85-5D, Elantrine, mixts. with hetrazepine derivative PAF antagonists 1242-69-9D, Decitropine, mixts. with hetrazepine derivative PAF antagonists 1329-38-0D, Alin, mixts. with hetrazepine derivative PAF antagonists 1508-75-4D, Tropicamide, mixts. with hetrazepine derivative PAF antagonists 1982-37-2D, Methdilazine, mixts. with hetrazepine derivative PAF antagonists 2090-54-2D, Aprobit, mixts. with hetrazepine derivative PAF antagonists 2681-10-9D, Fluoxyphenonium bromide, mixts. with hetrazepine derivative PAF antagonists 2870-71-5D, Hyoscyamine methyl bromide, mixts. with

hetrazepine derivative PAF antagonists 3166-62-9D, Methylbenactyzium bromide, mixts. with hetrazepine derivative PAF antagonists 3485-62-9D, Clidinium bromide, mixts. with hetrazepine derivative PAF antagonists 3569-58-2D, Oxysonium iodide, mixts. with hetrazepine derivative PAF antagonists 3569-59-3D, Hexasonium iodide, mixts. with hetrazepine derivative PAF antagonists 3612-98-4D, Troxypyrrolium tosylate, mixts. with hetrazepine derivative PAF antagonists 3614-30-0D, Emepronium bromide, mixts. with hetrazepine derivative PAF antagonists 3626-03-7D, Ethpenal, mixts. with hetrazepine derivative PAF antagonists 3690-58-2D, Fubrogonium iodide, mixts. with hetrazepine derivative PAF antagonists 3691-21-2D, Acemydrite, mixts. with hetrazepine derivative PAF antagonists 3735-90-8D, Fencarbamide, mixts. with hetrazepine derivative PAF antagonists 3811-12-9D, Mespenal, mixts. with hetrazepine derivative PAF antagonists 4047-34-1D, Trantelinium bromide, mixts. with hetrazepine derivative PAF antagonists 4310-35-4D, mixts. with hetrazepine derivative PAF antagonists 4354-45-4D, Oxyclipine, mixts. with hetrazepine derivative PAF antagonists 4425-78-9D, Aminocarbofluorene, mixts. with hetrazepine derivative PAF antagonists 4438-22-6D, Atropine oxide, mixts. with hetrazepine derivative PAF antagonists 4546-39-8D, Pipethanate, mixts. with hetrazepine derivative PAF antagonists 4630-95-9D, Prifinium bromide, mixts. with hetrazepine derivative PAF antagonists 4969-02-2D, Metixene, mixts. with hetrazepine derivative PAF antagonists 5205-82-3D, Bevonium methyl sulfate, mixts. with hetrazepine derivative PAF antagonists 5585-94-4D, Promandeline 263, mixts. with hetrazepine derivative PAF antagonists 5633-20-5D, Oxybutynin, mixts. with hetrazepine derivative PAF antagonists 5634-41-3D, mixts. with hetrazepine derivative PAF antagonists 5668-06-4D, Mecloxamine, mixts. with hetrazepine derivative PAF antagonists 5835-72-3D, Diprofene, mixts. with hetrazepine derivative PAF antagonists 5843-82-3D, mixts. with hetrazepine derivative PAF antagonists 5868-06-4D, Fentonium bromide, mixts. with hetrazepine derivative PAF antagonists 6043-01-2D, Domazoline, mixts. with hetrazepine derivative PAF antagonists 6191-48-6D, Barbetonii iodidum, mixts. with hetrazepine derivative PAF antagonists 6620-60-6D, Proglumide, mixts. with hetrazepine derivative PAF antagonists 6878-98-4, Tropacine 7009-54-3D, Pentapiperide, mixts. with hetrazepine derivative PAF antagonists 7009-76-9D, Triclazate, mixts. with hetrazepine derivative PAF antagonists 7219-91-2D, Thihexinol methyl bromide, mixts. with hetrazepine derivative PAF antagonists 7247-57-6D, Heteronium bromide, mixts. with hetrazepine derivative PAF antagonists 7638-50-8D, Oxyphenhydrazonium bromide, mixts. with hetrazepine derivative PAF antagonists 10139-98-7D, Deptropine methobromide, mixts. with hetrazepine derivative PAF antagonists 10405-02-4D, Trospium chloride, mixts. with hetrazepine derivative PAF antagonists 13118-09-7D, Hexapyrronium bromide, mixts. with hetrazepine derivative PAF antagonists 14007-64-8D, Butetamate, mixts. with hetrazepine derivative PAF antagonists 14051-33-3D, Benzetimide, mixts. with hetrazepine derivative PAF antagonists 14319-87-0D, mixts. with hetrazepine derivative PAF antagonists 14334-40-8D, Pramiverine, mixts. with hetrazepine derivative PAF antagonists 14617-17-5D, Triperiden, mixts. with hetrazepine derivative PAF antagonists 14745-50-7D, Meletimide, mixts. with hetrazepine derivative PAF antagonists 15130-91-3D, Sultroponium, mixts. with hetrazepine derivative PAF antagonists 15291-75-5D, BN 52020, mixts. with anticholinergics 15291-76-6D, BN 52022, mixts. with anticholinergics 15291-77-7D, BN 52021, mixts. with anticholinergics 15351-05-0D, Buzepide methiodide, mixts. with hetrazepine derivative PAF antagonists 15585-88-3D, Dicarfen, mixts. with hetrazepine derivative PAF antagonists 15790-02-0D, Tropodifene, mixts. with hetrazepine derivative PAF antagonists 15793-40-5D, Terodiline, mixts. with hetrazepine derivative PAF antagonists 17010-68-3D, Benzomethamine, mixts. with hetrazepine derivative PAF antagonists 17616-19-2D, Sch 221, mixts. with hetrazepine derivative PAF antagonists 17692-23-8D, Bentipimine, mixts. with hetrazepine derivative PAF antagonists

19410-02-7D, Tropirine, mixts. with hetrazepine derivative PAF antagonists 20448-86-6D, Bornaprine, mixts. with hetrazepine derivative PAF antagonists 21216-78-4D, Anacolin, mixts. with hetrazepine derivative PAF antagonists 21888-98-2, Dexetimide 22150-28-3D, Ipragratine, mixts. with hetrazepine derivative PAF antagonists 22235-85-4D, Naltropine, mixts. with hetrazepine derivative PAF antagonists 22254-24-6D, Atrovent, mixts. with hetrazepine derivative PAF antagonists 22487-42-9D, Benaprizine, mixts. with hetrazepine derivative PAF antagonists 23182-46-9D, mixts. with hetrazepine derivative PAF antagonists 24622-72-8D, Amixetrine, mixts. with hetrazepine derivative PAF antagonists 25314-87-8D, Elucaine, mixts. with hetrazepine derivative PAF antagonists 28810-23-3D, Zepastine, mixts. with hetrazepine derivative PAF antagonists 28911-01-5D, Triazolam, mixts. with anticholinergics 28981-97-7D, Alprazolam, mixts. with anticholinergics 29025-14-7D, Butropium bromide, mixts. with hetrazepine derivative PAF antagonists 29125-56-2D, Droclidinium bromide, mixts. with hetrazepine derivative PAF antagonists 29546-59-6D, Ciclonium bromide, mixts. with hetrazepine derivative PAF antagonists 30286-75-0D, Oxitropium bromide, mixts. with hetrazepine derivative PAF antagonists 35035-05-3D, Timepidium bromide, mixts. with hetrazepine derivative PAF antagonists 40455-41-2D, derivs., mixts. with anticholinergics 40759-33-9D, Nolinium bromide, mixts. with hetrazepine derivative PAF antagonists 42399-41-7D, mixts. with anticholinergics 47467-79-8D, Despasmin, mixts. with hetrazepine derivative PAF antagonists 50655-20-4D, FR 106969, mixts. with anticholinergics 51598-60-8D, Cimetropium bromide, mixts. with hetrazepine derivative PAF antagonists 52080-56-5D, Endobenzyline bromide, mixts. with hetrazepine derivative PAF antagonists 53716-44-2D, Rociverine, mixts. with hetrazepine derivative PAF antagonists 54063-52-4D, Pitofenone, mixts. with hetrazepine derivative PAF antagonists 55837-29-1D, Tiropramide, mixts. with hetrazepine derivative PAF antagonists 55869-99-3D, Anisodamine, mixts. with hetrazepine derivative PAF antagonists 57801-81-7D, Brotizolam, mixts. with anticholinergics 58493-54-2D, Ritropirronium bromide, mixts. with hetrazepine derivative PAF antagonists 65154-06-5D, PAF, antagonists, mixts. with anticholinergics 74149-38-5D, FR 49175, mixts. with anticholinergics 80387-96-8D, Difemerine, mixts. with hetrazepine derivative PAF antagonists 93363-02-1D, RP 52770, mixts. with anticholinergics 93363-11-2D, RP 48740, mixts. with anticholinergics 95851-37-9D, Kadsurenone, mixts. with anticholinergics 99103-35-2D, L 652731, mixts. with anticholinergics 99659-62-8D, ONO 6240, mixts. with anticholinergics 100488-87-7D, Cv 6209, mixts. with anticholinergics 101394-50-7D, L 653150, mixts. with anticholinergics 101706-33-6D, FR 900452, mixts. with anticholinergics 102841-48-5D, mixts. with anticholinergics 102841-49-6D, mixts. with anticholinergics 106556-34-7D, mixts. with anticholinergics 107438-79-9D, BN 52024, mixts. with anticholinergics 109516-82-7D, Sri 63.675, mixts. with anticholinergics 111372-42-0D, LG 50643, mixts. with anticholinergics 113787-28-3D, L 659989, mixts. with anticholinergics 115622-31-6D, Sdz 64.412, mixts. with anticholinergics 116289-53-3D, RP 59227, mixts. with anticholinergics 117075-96-4D, RU 45703, mixts. with anticholinergics 117279-73-9D, Y 24180, mixts. with anticholinergics 117796-52-8D, Sch 37370, mixts. with anticholinergics 118196-11-5D, Ym 461, mixts. with anticholinergics 120889-14-7D, BN 52111, mixts. with anticholinergics 120908-94-3D, BN 52115, mixts. with anticholinergics 122956-68-7D, Uk 74505, mixts. with anticholinergics 123875-01-4D, Pca 4248, mixts. with anticholinergics 125030-71-9D, mixts. with anticholinergics 125372-33-0D, RP 55778, mixts. with anticholinergics 127279-06-5D, BN 50726, mixts. with anticholinergics 128420-61-1D, e 5880, mixts. with anticholinergics 128672-07-1D, BN 50739, mixts. with anticholinergics 130841-70-2D, Sm 10661, mixts. with anticholinergics **131311-25-6D** , Tcv 309, mixts. with anticholinergics 131614-02-3D, E 6123, mixts.

with anticholinergics 131888-54-5D, Ym 264, mixts. with anticholinergics 132418-35-0D, BN 50727, mixts. with anticholinergics 132579-32-9D, BN 50730, mixts. with anticholinergics 135947-75-0D, MK 287, mixts. with anticholinergics 136408-45-2D, Ur 10324, mixts. with anticholinergics 138060-13-6D, Ur 11353, mixts. with anticholinergics 143445-03-8D, L 668750, mixts. with anticholinergics 147517-17-7D, Y 20411, mixts. with anticholinergics 147769-54-8D, derivs., mixts. with anticholinergics 147769-55-9D, derivs., mixts. with anticholinergics 150769-93-0D, BN 50580, mixts. with anticholinergics 150769-94-1D, BN 50585, mixts. with anticholinergics 150769-95-2D, BN 50766, mixts. with anticholinergics 150769-96-3D, BN 52023, mixts. with anticholinergics 150769-97-4D, BN 52025, mixts. with anticholinergics 150769-98-5D, BN 54068, mixts. with anticholinergics 150770-06-2D, Cn 3988, mixts. with anticholinergics 150770-23-3D, F 1850, mixts. with anticholinergics 150770-56-2D, R 74654, mixts. with anticholinergics 150770-59-5D, RN 70727, mixts. with anticholinergics 150770-61-9D, RP 55270, mixts. with anticholinergics 150770-66-4D, Sri 441, mixts. with anticholinergics 153478-75-2D, mixts. with hetrazepine derivative PAF antagonists 153550-04-0D, Amphiolen, mixts. with hetrazepine derivative PAF antagonists 153550-49-3D, Oxident, mixts. with hetrazepine derivative PAF antagonists
RL: BIOL (Biological study)
(drugs for treatment of bronchial asthma, synergistic)

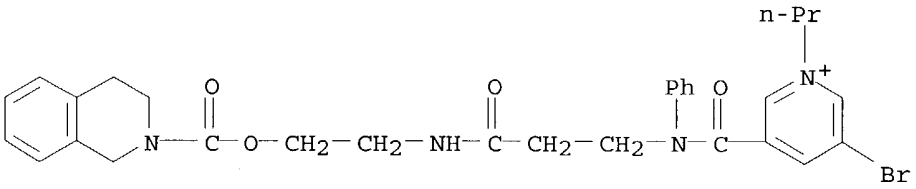
IT **131311-25-6D**, Tcv 309, mixts. with anticholinergics
RL: BIOL (Biological study)
(drugs for treatment of bronchial asthma, synergistic)

RN 131311-25-6 HCAPLUS

CN Pyridinium, 3-bromo-5-[[[3-[[2-[[(3,4-dihydro-2(1H)-isoquinolinyl)carbonyl]oxy]ethyl]amino]-3-oxopropyl]phenylamino]carbonyl]-1-propyl-, nitrate (9CI) (CA INDEX NAME)

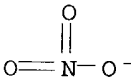
CM 1

CRN 131311-24-5
CMF C30 H34 Br N4 O4



CM 2

CRN 14797-55-8
CMF N O3



L42 ANSWER 45 OF 101 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1993:610708 HCAPLUS

DN 119:210708
ED Entered STN: 13 Nov 1993
TI Treatment of dysmenorrhea with PAF antagnoists
IN Kutter, Eberhard
PA Boehringer Ingelheim KG, Germany
SO Ger. Offen., 8 pp.
CODEN: GWXXBX
DT **Patent**
LA German
IC ICM A61K031-55
CC 63-5 (Pharmaceuticals)
Section cross-reference(s): 28
FAN.CNT 1

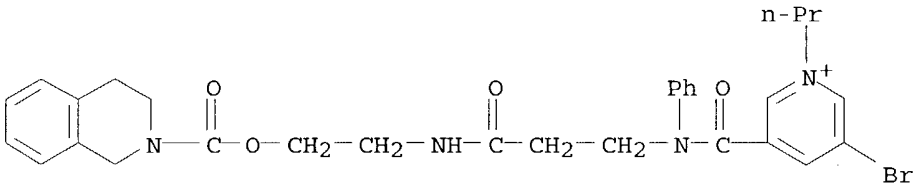
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 4200610	A1	19930715	DE 1992-4200610	19920113 <--
	WO 9313776	A1	19930722	WO 1993-EP47	19930112 <--

W: JP, US
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE
PRAI DE 1992-4200610 19920113 <--
OS MARPAT 119:210708
AB PAF antagonists are drugs for the treatment of dysmenorrhea, especially primary dysmenorrhea (no data). Suitable PAF antagonists are alprazolam, dilthiazem, brotizolam, hetrazepine derivs., etc. Formulation examples are given. The PAF antagonist 2-[4-(2-chlorophenyl)-9-methyl-6H-thieno[3,2-f][1,2,4]triazolo[4,3-a][1,4]diazepin-2-yl]ethane-1-carboxylic acid morpholide was prepared by the reaction of 2-[4-(2-chlorophenyl)-9-methyl-6H-thieno[3,2-f][1,4]diazepin-2-yl]ethane-1-carboxylic acid with N-hydroxybenzotriazole and morpholine, in absolute DMF.
ST dysmenorrhea drug PAF antagonist; thiazolodiazepine deriv prepn drug
IT Dysmenorrhea
(treatment of, with PAF antagonist)
IT 15291-75-5, BN-52020 15291-76-6, BN-52022 15291-77-7, BN-52021 28911-01-5, Triazolam 28981-97-7, Alprazolam 42399-41-7 50655-20-4, FR-106969 57801-81-7, Brotizolam 74149-38-5, FR-49175 93363-02-1, RP-52770 93363-11-2, RP-48740 95851-37-9 99103-35-2, L-652731 99659-62-8, ONO-6240 100488-87-7, CV-6209 101394-50-7, L-653150 101706-33-6, FR-900452 102841-48-5 102841-49-6 106556-34-7 107438-79-9, BN 52024 109516-82-7 111372-42-0, LG 50643 113787-28-3, L-659989 114776-28-2, WEB-2170 115622-31-6 116289-53-3, RP-59227 117075-96-4, RU-45703 117279-73-9, Y-24180 117796-52-8, SCH-37370 118196-11-5, YM-461 120889-14-7, BN-52111 120908-94-3, BN-52115 122956-68-7, UK-74505 123875-01-4, PCA-4248 125030-71-9 125372-33-0, RP-55778 127279-06-5, BN-50726 128420-61-1, E-5880 128672-07-1, BN-50739 130841-70-2, SM-10661 **131311-25-6**, TCV-309 131614-02-3, E-6123 131888-54-5, YM-264 132418-35-0, BN-50727 132579-32-9, BN-50730 135947-75-0, MK-287 136408-45-2, UR-10324 138060-13-6, UR-11353 143445-03-8, L-668750 147517-17-7, Y-20411 150769-93-0, BN 50580 150769-94-1, BN 50585 150769-95-2, BN 50766 150769-96-3, BN 52023 150769-97-4, BN 52025 150769-98-5, BN 54068 150770-06-2, CN 3988 150770-23-3, F 1850 150770-56-2, R 74654 150770-59-5, RN 70727 150770-61-9, RP 55270 150770-66-4, SRI 441
RL: BIOL (Biological study)
(PAF antagonist, dysmenorrhea treatment by)
IT 40455-41-2D, derivs. 147769-54-8D, derivs. 150677-76-2D, derivs.
RL: BIOL (Biological study)
(PAF antagonists, dysmenorrhea treatment by)
IT 65154-06-5, Blood platelet-activating factor
RL: BIOL (Biological study)
(antagonist of, as drugs for treatment of dysmenorrhea)

IT 105219-56-5P
RL: PREP (Preparation)
(preparation of, as PAF antagonist, for treatment of dysmenorrhea)
IT 100826-98-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with hydroxybenzotriazole and morpholine)
IT 110-91-8, Morpholine, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with thienodiazepine derivative and hydroxybenzothiazole)
IT 2592-95-2, N-Hydroxybenzotriazole
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with thienodiazepine derivative and morpholine)
IT **131311-25-6**, TCV-309
RL: BIOL (Biological study)
(PAF antagonist, dysmenorrhea treatment by)
RN 131311-25-6 HCAPLUS
CN Pyridinium, 3-bromo-5-[[[3-[[2-[[(3,4-dihydro-2(1H)-isoquinolinyl)carbonyl]oxy]ethyl]amino]-3-oxopropyl]phenylamino]carbonyl]-1-propyl-, nitrate (9CI) (CA INDEX NAME)

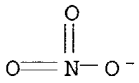
CM 1

CRN 131311-24-5
CMF C30 H34 Br N4 O4



CM 2

CRN 14797-55-8
CMF N O3

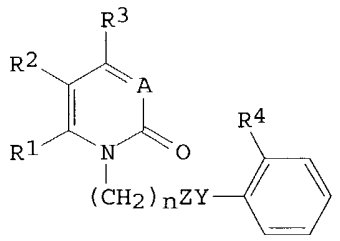


L42 ANSWER 50 OF 101 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1992:651364 HCAPLUS
DN 117:251364
ED Entered STN: 26 Dec 1992
TI Preparation of [(carboxybiphenylyl)methyl]pyridones, -pyrimidones, and related compounds as angiotensin II receptor blockers
IN Bantick, John Raymond; McInally, Thomas; Tinker, Alan Charles; Hirst, Simon Christopher
PA Fisons PLC, UK
SO Eur. Pat. Appl., 39 pp.
CODEN: EPXXDW
DT **Patent**

LA English
IC ICM C07D239-36
ICS C07D213-64; C07D213-69; C07D213-80; C07D213-82; C07D215-22; C07D401-10; C07D401-12; C07D403-10; C07D405-06; C07D405-14
CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 27
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
PI	EP 500297	A1	19920826	EP 1992-301283	19920217	<--
	R: PT					
	ZA 9201022	A	19930127	ZA 1992-1022	19920212	<--
	CN 1068109	A	19930120	CN 1992-101623	19920214	<--
	CA 2104108	AA	19920817	CA 1992-2104108	19920217	<--
	WO 9214714	A1	19920903	WO 1992-GB280	19920217	<--
	W: AU, BR, CA, CS, DK, FI, HU, JP, KR, NO, PL, RU, US					
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, MC, NL, SE					
	AU 9212287	A1	19920915	AU 1992-12287	19920217	<--
	EP 572455	A1	19931208	EP 1992-904509	19920217	<--
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE					
	JP 06505715	T2	19940630	JP 1992-504196	19920217	<--
PRAI	GB 1991-3326		19910216	<--		
	GB 1991-12975		19910615	<--		
	GB 1991-13492		19910621	<--		
	GB 1991-14829		19910710	<--		
	GB 1991-20677		19910928	<--		
	GB 1991-24168		19911114	<--		
	GB 1991-25059		19911126	<--		
	GB 1991-26573		19911212	<--		
	GB 1991-26575		19911212	<--		
	GB 1992-101		19920104	<--		
	WO 1992-GB280		19920217	<--		

OS MARPAT 117:251364
GI



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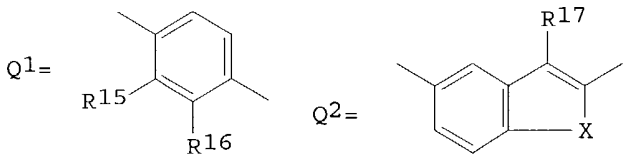
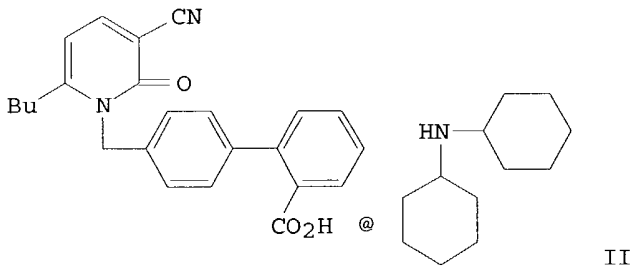




II

AB Title compds. [I; A = N, CR5; R2 = H, alkyl, halo, CO2R21; R1R2 = B:CR7CR8:CR9; B = N, CR6; R6-R9 = H, alkyl, alkoxy, SOqR22, CO2R23; R3 = H, OH, alkyl, alkoxy, (CH2)rCO2R10, (CH2)tR31, amino; R5 = H, alkyl, alkanoyl, Ph, halo, cyano, NO2, amino, CONR11R12, (CH2)mOR13, CO2R14; Z = Q1, Q2; X = O, S, imino; Y = (CH2)s, OCHR20, SCHR20, NR28CO; R10, R14 = H, alkyl, Ph, phenylalkyl, (diphenylmethyl)alkyl; one of R4, R20 = CO2H, tetrazolyl, the other = H; R22 = alkyl; R11, R13, R21, R23, R28, R31 = H, alkyl; R11R12 = CH2CH2MCH2CH2; M = O, imino; n, m = 1-6; q = 0-2; r, s, t = 0-6], were prepared as angiotensin II receptor blockers (no data). Thus, 6-butyl-3-cyano-2(1H)-pyridone and Me 4'-bromomethyl-1,1'-biphenyl-2-carboxylate were coupled using NaH in DMF; the product was saponified with LiOH followed by conversion to the dicyclohexylamine salt II.

ST biphenylylmethylpyridone angiotensin II receptor blocker; pyridone carboxybiphenylylmethyl angiotensin receptor blocker; quinolone tetrazolylbiphenylylmethyl angiotensin receptor blocker

IT 11128-99-7, Angiotensin II
RL: RCT (Reactant); RACT (Reactant or reagent)
([(carboxybiphenylyl)methyl]pyridones, -pyrimidones, and related compds.)

IT 144457-68-1P 144457-69-2P 144457-70-5P 144457-71-6P 144457-72-7P
144457-73-8P 144457-74-9P **144457-75-0P** 144457-76-1P
144457-77-2P 144457-78-3P 144457-79-4P 144457-80-7P 144457-81-8P
144457-82-9P 144457-83-0P 144457-84-1P 144457-85-2P
144457-86-3P 144457-87-4P 144457-88-5P 144457-89-6P 144457-90-9P
144457-91-0P 144457-92-1P 144457-93-2P 144457-94-3P 144457-95-4P
144457-96-5P 144457-97-6P 144457-98-7P 144457-99-8P 144458-00-4P
144458-01-5P 144458-02-6P 144458-03-7P 144458-04-8P 144458-05-9P
144458-06-0P 144458-07-1P 144458-08-2P 144458-09-3P 144458-10-6P
144458-11-7P 144458-12-8P 144458-13-9P 144458-14-0P 144458-15-1P
144458-16-2P 144458-17-3P 144458-18-4P 144458-19-5P 144705-81-7P

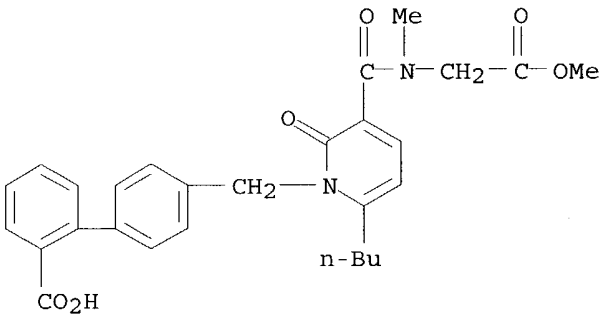
144705-82-8P 144705-83-9P 144705-85-1P 144705-86-2P 144705-87-3P
144705-93-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as angiotensin II receptor blocker)

IT 137863-75-3P 137863-76-4P 143381-85-5P 144458-20-8P 144458-21-9P
144458-22-0P 144458-23-1P 144458-24-2P 144458-25-3P 144458-26-4P
144458-27-5P 144458-28-6P 144458-29-7P 144458-30-0P 144458-31-1P
144458-32-2P 144458-33-3P 144458-34-4P 144458-35-5P 144458-36-6P
144458-37-7P 144458-38-8P 144458-39-9P 144458-40-2P 144458-41-3P
144458-42-4P 144458-43-5P 144458-44-6P 144458-45-7P 144458-46-8P
144458-47-9P 144458-48-0P 144458-49-1P 144458-50-4P 144458-51-5P
144458-52-6P 144458-53-7P 144458-54-8P 144458-55-9P 144458-56-0P
144458-57-1P 144458-58-2P 144458-59-3P 144458-60-6P 144458-61-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for angiotensin II receptor blocker)

IT 83-13-6, Diethyl phenylmalonate 103-80-0, Phenylacetyl chloride
1118-03-2, Trimethylstannyl azide 1738-68-7, Glycine benzyl ester
2916-68-9 3249-68-1, Ethyl 3-oxohexanoate 5348-51-6,
2-Hydroxy-4-methylpyrimidine hydrochloride 7148-03-0 14818-55-4
14818-57-6 18742-94-4 36239-09-5, Ethyl malonyl chloride 39619-07-3,
Methyl malonyl dichloride 53277-47-7 66181-56-4 83499-38-1
91822-41-2 114772-38-2 114772-54-2 118420-86-3 133052-21-8
133690-92-3 143381-83-3 144458-25-3 144458-32-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in preparation of angiotensin II receptor blocker)

IT **144457-75-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as angiotensin II receptor blocker)

RN 144457-75-0 HCAPLUS
CN [1,1'-Biphenyl]-2-carboxylic acid, 4'-[[6-butyl-3-[[(2-methoxy-2-oxoethyl)methylamino]carbonyl]-2-oxo-1(2H)-pyridinyl]methyl]- (9CI) (CA INDEX NAME)

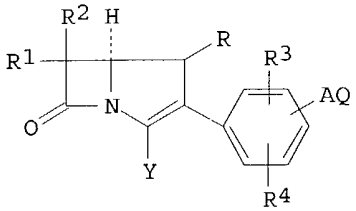


L42 ANSWER 55 OF 101 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1991:247040 HCAPLUS
DN 114:247040
ED Entered STN: 28 Jun 1991
TI Preparation of 2-[pyridinium-1-ylmethyl)phenyl]carbapenems and analogs as antibiotics
IN DiNinno, Frank P.; Muthard, David A.; Salzmann, Thomas N.
PA Merck and Co., Inc., USA
SO U.S., 20 pp. Cont.-in-part of U.S. Ser. No. 9,865, abandoned.
CODEN: USXXAM
DT **Patent**
LA English

IC ICM C07D487-04
ICS A61K031-40
NCL 514210000
CC 26-5 (Biomolecules and Their Synthetic Analogs)
Section cross-reference(s): 1
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4978659	A	19901218	US 1989-396165	19890821 <--
	CA 1322002	A1	19930907	CA 1988-557787	19880201 <--
	JP 01197483	A2	19890809	JP 1988-22656	19880202 <--
	JP 06084376	B4	19941026		
PRAI	US 1987-9865		19870202 <--		

OS MARPAT 114:247040
GI



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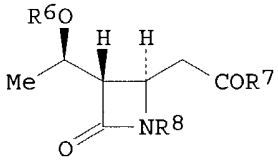
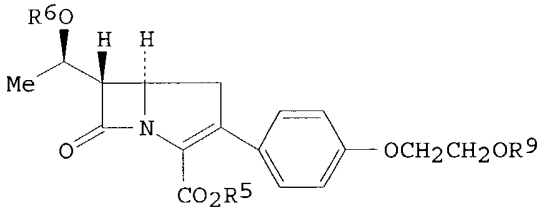


II

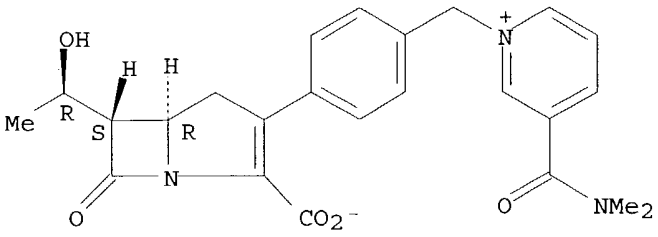


IV

AB The title compds. [I; A = (CH2)mZ(CH2)n; Q = substituted pyridinium-1-yl and analogous cyclic ammonium groups; R = H, Me; R1, R2 = H, Me, Et, HOCH2, MeCH(OH), Me2C(OH), FCH2CH(OH), F2CHCH(OH), F3CCH(OH), MeCHF, MeCF2, Me2CF; R3,R4 = CF3, halo, OH, alkoxy, NH2, etc.; Y = CO2R5; R5 = neg. charge, pharmaceutically acceptable ester residue or cation; Z = bond, O, SOp, (alkyl)imino; m, p-0-2; n = 1,2] were prepared as antibiotics (no data). Thus, 4-BrC6H4OCH2CH2OSiMe2CMe3 was condensed with azetidinone derivative II [R6 = CH2:CHCH2O2C, R8 = C(:PPh3)CO2CH2CH:CH2] (III; R7 = pyridylthio) to give III (R7 = C6H4OCH2CH2OSiMe2CMe3) which was refluxed with hydroquinone in xylene to give carbapenemcarboxylate IV (R5 = CH2CH:CH2, R6 = CH2:CHCH2O2C, R9 = H) which was stirred 15 min at 0° with (CF3SO2)2O and 4-dimethylaminopyridine in CH2Cl2 to give, after deprotection, IV (R5 = neg. charge, R6 = H, R9 = 4-dimethylaminopyridinium-1-yl).
ST carbapenem pyridiniumylmethylphenyl prepn antibiotic
IT Antibiotics
((pyridiniumylmethyl)phenylcarbapenems and analogs)
IT 358-23-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(esterification of, with (hydroxybenzyl)carbapenem derivative)
IT 119922-80-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(mesylation of)

IT 119890-97-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and conversion to iodide derivative)
IT 119890-99-2P 119891-02-0P 119891-04-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deprotection of)
IT 119890-98-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and quaternization by, of pyridine derivative)
IT 133305-44-9P 133305-45-0P 133305-46-1P 133305-48-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of antibiotics)
IT 119891-00-8P 119891-05-3P 119891-06-4P 119891-07-5P 119891-08-6P
119891-09-7P 119891-10-0P **119891-11-1P** 119891-12-2P
119891-13-3P 119891-14-4P 119891-15-5P 119891-16-6P 119891-17-7P
119891-18-8P 119891-19-9P 119891-20-2P 119891-21-3P 119891-22-4P
119891-23-5P 119922-81-5P 120764-70-7P 120764-71-8P 120764-72-9P
121395-65-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of, as antibacterial)
IT 133305-49-4P 133305-50-7P 133305-51-8P 133305-52-9P 133305-53-0P
133305-54-1P 133305-55-2P 133305-56-3P 133305-57-4P 133305-58-5P
133305-59-6P 133305-60-9P 133305-61-0P 133305-62-1P 133305-63-2P
133305-64-3P 133305-65-4P 133305-66-5P 133305-67-6P 133305-68-7P
133305-69-8P 133338-03-1P 133397-79-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of, as antibiotic)
IT 100-54-9, 3-Pyridinecarbonitrile 462-08-8, 3-Pyridinamine
RL: RCT (Reactant); RACT (Reactant or reagent)
(quaternization of, by carbapenem derivative)
IT 1122-58-3, 4-Dimethylaminopyridine 133305-43-8 133329-99-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in preparation of antibiotics)
IT **119891-11-1P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of, as antibacterial)
RN 119891-11-1 HCAPLUS
CN Pyridinium, 1-[[4-[2-carboxy-6-(1-hydroxyethyl)-7-oxo-1-azabicyclo[3.2.0]hept-2-en-3-yl]phenyl]methyl]-3-[(dimethylamino)carbonyl]-, inner salt, [5R-[5α,6α(R*)]]- (9CI) (CA INDEX NAME)

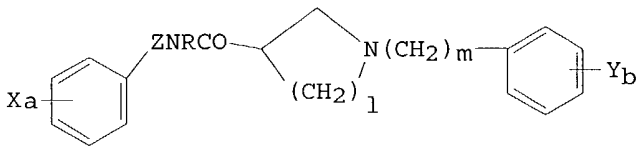
Absolute stereochemistry.



L42 ANSWER 60 OF 101 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1990:591179 HCAPLUS
DN 113:191179
ED Entered STN: 23 Nov 1990
TI Cyclic amine 3-carboxamide derivatives as cardiovascular agents
IN Sekiya, Tetsuo; Tsutsui, Mikio; Kikuchi, Junko; Horii, Daijiro; Ishibashi, Akira; Suzuki, Junko
PA Mitsubishi Kasei Corp., Japan
SO Jpn. Kokai Tokkyo Koho, 11 pp.
CODEN: JKXXAF
DT **Patent**
LA Japanese
IC ICM C07D207-16
ICS C07D211-60; C07D405-12
ICA A61K031-40; A61K031-445
CC 27-16 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI JP 02138170	A2	19900528	JP 1988-293111	19881119 <--
PRAI JP 1988-293111		19881119 <--		

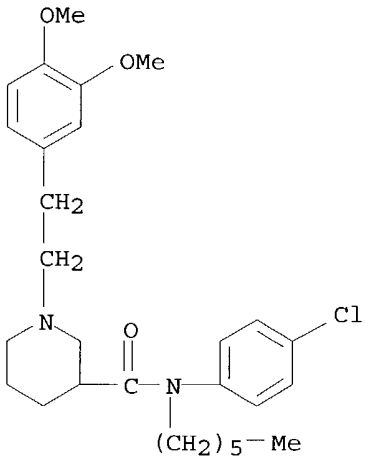
OS MARPAT 113:191179
GI



I

AB The title derivs. I (R = H, linear or branched C1-8 alkyl; X, Y = H, C1-5 alkyl, C1-5 alkoxy, halo, OCH2O, OCH2CH2O; Z = linear or branched C1-5 alkylene; a, b = 1-3; l = 2-4; m = 2-5) and their pharmacol. acceptable salts, showing antitachycardiac and vasodilatory activity and useful for treatment of arrhythmia, angina pectoris, hypertension, etc., are prepared DCC was added dropwise to a CH2Cl2 solution of N-(3,4-dimethoxyphenethyl)nipecotic acid at 0° and the mixture was further stirred at room temperature for 1 h, after addition of 3,4-(MeO)2C6H3CH2CH2NH2, the reaction mixture was stirred at room temperature overnight to give 47.7% 1-(3,4-dimethoxyphenethyl)-3-(3,4-dimethoxyphenethylaminocarbonyl)piperidine. This lowered isoproterenol-induced increased heart beat rate of atrium isolated from guinea pig at ED30 (a concentration of drug lowering heart beat rate by 30%) 1.8 μM, vs. 3.0 μM for 2-[N-methyl-N-(3,4-

dimethoxyphenethyl)aminopropyl]-5,6-dimethoxyphthalimidin-1-one.
ST nipecotamide deriv prepn cardiovascular agent; antiarrhythmic phenethylnipecotamide deriv prepn; vasodilator phenethylnipecotamide deriv prepn; tachycardia treatment phenethylnipecotamide deriv prepn; angina pectoris treatment phenethylnipecotamide prepn; antihypertensive phenethylnipecotamide deriv prepn
IT Antihypertensives
Vasodilators
([(phenylalkyl)aminocarbonyl]-N-(phenylalkyl)piperidines)
IT Antiarrhythmics
([(phenylalkyl)aminocarbonyl]-N-phenylalkyl-cyclic amines)
IT Heart, disease or disorder
(angina pectoris, treatment of, [(phenylalkyl)aminocarbonyl]-N-(phenylalkyl)piperidines for)
IT Heart, disease or disorder
(tachycardia, treatment of, [(phenylalkyl)aminocarbonyl]-N-(phenylalkyl)piperidines for)
IT 129597-73-5 129597-74-6 129597-75-7 129597-76-8 129597-77-9
129597-78-0 129597-79-1 129597-80-4 129597-81-5 129597-82-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(amidation of, with phenethylamines)
IT 64-04-0, Benzeneethanamine 120-20-7, 3,4-Dimethoxyphenethylamine
156-41-2, 4-Chlorophenethylamine 1484-85-1, 3,4-Methylenedioxyphenethylamine 2045-79-6, 2-Methoxyphenethylamine
3213-28-3, 3,5-Dimethoxyphenethylamine 10554-64-0, 3,4-Ethylenedioxyphenethylamine 21581-45-3, 3,4-Dichlorophenethylamine
67851-51-8, 3,5-Dichlorophenethylamine 73918-56-6, 4-Bromophenethylamine
84558-03-2, 4-Isopropylphenethylamine 129597-85-9, N-(4-Chlorophenethyl)-N-hexylamine
RL: RCT (Reactant); RACT (Reactant or reagent)
(amidation with, of N-(phenylalkyl)nipecotic or pyrrolidinecarboxylic acids)
IT 129597-83-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as antitachycardiac and vasodilator)
IT 129597-87-1P 129597-88-2P 129597-89-3P 129597-90-6P 129597-91-7P
129597-92-8P 129597-93-9P 129597-94-0P 129597-95-1P 129597-96-2P
129597-97-3P 129597-98-4P 129597-99-5P 129598-00-1P 129598-01-2P
129598-02-3P 129598-03-4P **129598-04-5P** 129598-05-6P
129598-06-7P 129598-07-8P 129598-08-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as vasodilator and antitachycardiac agent)
IT 129597-86-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(N-alkylation of, with fluorophenethyl mesylate)
IT 130680-89-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(N-alkylation with, of (dimethoxyphenethylaminocarbonyl)piperidine)
IT **129598-04-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as vasodilator and antitachycardiac agent)
RN 129598-04-5 HCAPLUS
CN 3-Piperidinecarboxamide, N-(4-chlorophenyl)-1-[2-(3,4-dimethoxyphenyl)ethyl]-N-hexyl- (9CI) (CA INDEX NAME)



L42 ANSWER 65 OF 101 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1989:533992 HCAPLUS
DN 111:133992
ED Entered STN: 14 Oct 1989
TI Pyridinium derivatives and their production, pharmaceutical compositions, and use as antagonists of platelet activating factor
IN Tsushima, Susumu; Takatani, Muneo; Nishikawa, Kohei
PA Takeda Chemical Industries, Ltd., Japan
SO Eur. Pat. Appl., 164 pp.
CODEN: EPXXDW
DT **Patent**
LA English
IC ICM C07D213-82
ICS C07D215-54; C07D401-12; A61K031-455; A61K031-47
CC 27-16 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1
FAN.CNT 1

	PATENT NO.	KIND	DATE		APPLICATION NO.	DATE	
PI	EP 301751	A1	19890201		EP 1988-306622	19880720	<--
	EP 301751	B1	19930310				
	R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE						
	AT 86614	E	19930315		AT 1988-306622	19880720	<--
	ZA 8805304	A	19900328		ZA 1988-5304	19880721	<--
	IL 87189	A1	19960723		IL 1988-87189	19880722	<--
	JP 02076854	A2	19900316		JP 1988-186494	19880725	<--
	JP 2756975	B2	19980525				
	US 4962113	A	19901009		US 1988-224352	19880726	<--
	AU 8820101	A1	19890209		AU 1988-20101	19880727	<--
	AU 613653	B2	19910808				
	DK 8804214	A	19890201		DK 1988-4214	19880728	<--
	CA 1339645	A1	19980127		CA 1988-573439	19880729	<--
	KR 125929	B1	19971226		KR 1988-9705	19880730	<--
PRAI	JP 1987-193479	A	19870731	<--			
	JP 1988-138908	A	19880606	<--			
	EP 1988-306622	A	19880720	<--			

OS MARPAT 111:133992
GI For diagram(s), see printed CA Issue.
AB Title compds. I [R1 = alkyl, aralkyl; R7, R10 = H, alkyl, aryl, aralkyl; l = 0, 1; R5 = (un)substituted C6H4 or alkylene; R11 = alkyl, aryl; X =

CH2OCH2, (CHR6)m; R6 = H, alkyl, alkoxy; m = 0-3; U = OCO, NR4CO, NR4SO2; R4 = H, alkyl, aryl, aralkyl; Y, Z = divalent chain containing 1-6 of O, NR, CO, S, and SO2, with ≥1 member being O or NR; R = H, alkyl, acyl, aryl; pyridine ring is optionally substituted; W- = counter anion; R may form ring with another R, R4, or R11] are prepared as antagonists of platelet activating factor (PAF). N-[2-(1,2,3,4-Tetrahydroisoquinolyl)carbonyloxyethyl]-3-anilinopropanamide (prepared in 4 steps) was condensed with 5-chloronicotinic acid chloride hydrochloride to give 63.0% of corresponding nicotinamide, which underwent quaternization by PrI and anion exchange on a resin to give 75.6% chloro-N,N-{[[[[(tetrahydroisoquinolyl)carbonyloxy]ethyl]carbamoyl]ethyl}{phenyl}carbamoyl(propyl)pyridinium chloride II. At 3 mg/kg orally in rats, 1 h prior to dosing with 1 μg/kg i.v. of PAF, II gave 93% inhibition of PAF-induced hypotension.

ST pyridinium prepn platelet activating factor antagonist; PAF antagonist pyridinium prepn

IT Allergy inhibitors
Antihypotensives
Bronchodilators
Inflammation inhibitors
(pyridinium salts)

IT 65154-06-5, Platelet activating factor
RL: RCT (Reactant); RACT (Reactant or reagent)
(inhibitors of, pyridinium salts as)

IT 93-20-9P 711-82-0P 2924-66-5P 21911-84-2P 26690-80-2P
46802-69-1P 50882-68-3P 57561-39-4P 60356-78-7P 73965-85-2P
96568-02-4P 106877-00-3P 106877-01-4P 106877-02-5P 106877-03-6P
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121493-58-1P 121493-60-5P 121493-61-6P 121493-63-8P 121493-65-0P
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121495-80-5P 121495-84-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in platelet activating factor-antagonizing pyridinium salts)

IT 121495-97-4P 121496-01-3P 121496-04-6P 121496-06-8P 121496-07-9P
121496-08-0P 121496-10-4P 121496-11-5P 121496-12-6P 121496-17-1P
121496-18-2P 121496-19-3P 121496-22-8P 121496-26-2P 121496-28-4P
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121496-46-6P 121496-47-7P 121496-49-9P 121496-51-3P 121496-53-5P
121496-55-7P 121496-56-8P 121516-00-5P 121519-98-0P 121519-99-1P
121520-00-1P 121520-01-2P 121520-51-2P 121520-56-7P 121520-57-8P
121520-58-9P 121520-59-0P 121520-62-5P 121520-63-6P 121520-64-7P
121520-65-8P 121520-67-0P 121520-75-0P 121520-76-1P 121524-29-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in platelet activating factor-antagonizing pyridinium salts)

IT 121493-43-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of platelet activating factor antagonist)

IT 121492-34-0P 121492-37-3P 121492-63-5P 121493-01-4P 121493-10-5P
121493-31-0P 121494-44-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of platelet activating factor-antagonizing pyridinium salts)

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121492-18-0P 121492-20-4P 121492-22-6P
121492-23-7P 121492-24-8P 121492-26-0P
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121492-33-9P 121492-35-1P 121492-36-2P
121492-38-4P 121492-39-5P 121492-42-0P
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121494-79-9P 121494-83-5P 121494-88-0P
121494-92-6P 121494-94-8P **121494-98-2P** 121495-01-0P
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121496-29-5P 121496-30-8P 121496-31-9P
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121496-35-3P 121496-36-4P 121496-41-1P
121496-43-3P 121496-45-5P **121496-48-8P**
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121520-55-6P 121520-60-3P 121520-61-4P
121520-66-9P 121520-68-1P **121520-69-2P**
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121520-73-8P 121520-74-9P 121541-31-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as platelet activating factor antagonist)

IT 62-53-3, Benzenamine, reactions 78-96-6, 1-Amino-2-propanol 79-04-9, Chloroacetyl chloride 79-22-1, Methyl chlorocarbonate 85-41-6, Phthalimide 85-46-1, 1-Naphthalenesulfonyl chloride 86-84-0, α-Naphthyl isocyanate 91-21-4, 1,2,3,4-Tetrahydroisoquinoline 93-11-8, 2-Naphthylsulfonyl chloride 98-88-4, Benzoyl chloride 100-46-9, Benzylamine, reactions 103-71-9, Phenyl isocyanate, reactions 104-63-2, N-Benzylethanolamine 107-15-3, 1,2-Ethanediamine, reactions 107-21-1, Ethylene glycol, reactions 108-31-6, 2,5-Furandione, reactions 109-83-1, N-Methylethanolamine 110-73-6, N-Ethylaminoethanol 110-89-4, Piperidine, reactions 110-91-8, Morpholine, reactions 111-26-2,

n-Hexylamine 111-36-4, Butyl isocyanate 111-75-1 112-96-9, Octadecyl isocyanate 118-31-0, 1-Naphthylmethylamine 122-98-5, β-Anilinoethanol 122-99-6, 2-Phenoxyethanol 124-22-1, 1-Aminododecane 134-32-7, 1-Naphthylamine 141-43-5, Monoethanolamine, reactions 156-87-6, 3-Aminopropanol 404-95-5 496-15-1, Indoline 503-38-8, Trichloromethyl chloroformate 525-03-1, 9-Aminofluorene 541-28-6, Isoamyl iodide 628-89-7, 2-(2-Chloroethoxy)ethanol 635-46-1, 1,2,3,4-Tetrahydroquinoline 636-73-7, 3-Pyridinesulfonic acid 638-45-9, Hexyl iodide 702-17-0 705-61-3, 2-Anilinopropionic acid 771-99-3, 4-Phenylpiperidine 879-18-5, 1-Naphthoyl chloride 929-06-6, 2-(2-Aminoethoxy)ethanol 1074-82-4 1195-45-5, 4-Fluorophenyl isocyanate 1622-32-8, 2-Chloroethanesulfonyl chloride 1664-40-0, N-Phenylethylenediamine 1885-14-9, Phenyl chlorocarbonate 2508-29-4, 5-Amino-1-pentanol 2759-28-6, N-Benzylpiperazine 2933-74-6 2933-76-8 2933-81-5 3055-93-4 3173-53-3, Cyclohexyl isocyanate 3303-84-2 4635-59-0, 4-Chlorobutyryl chloride 5197-62-6, 2-[2-(2-Chloroethoxy)ethoxy]ethanol 6168-72-5, DL-2-Amino-1-propanol 6393-19-7 7568-93-6, 2-Amino-1-phenylethanol 13214-66-9, 4-Phenylbutylamine 13325-10-5, 4-Amino-1-butanol 16369-21-4 20260-53-1, Nicotinic acid chloride hydrochloride 21617-14-1 24424-99-5, Di-tert-butyl dicarbonate 26734-09-8 30448-32-9 31121-11-6, 3-Anilinopropan-1-ol 33228-45-4, 4-Hexylaniline 36190-77-9 39178-35-3 39901-94-5, Picolinoyl chloride hydrochloride 39905-57-2, 4-Hexyloxyaniline 46802-69-1 55110-99-1 57823-20-8 59105-51-0 66608-11-5 66977-45-5 73339-01-2 82671-06-5, 2,6-Dichloro-5-fluoronicotinic acid 100487-92-1 100489-54-1 100489-90-5 111545-64-3, Quinoline-3-carboxylic acid chloride hydrochloride 121494-14-2 121494-81-3 121495-48-5 121495-51-0 121495-73-6 121495-75-8 121495-77-0 121495-78-1 121495-79-2 121496-16-0 121496-37-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in preparation of platelet activating factor-antagonizing pyridinium salts)

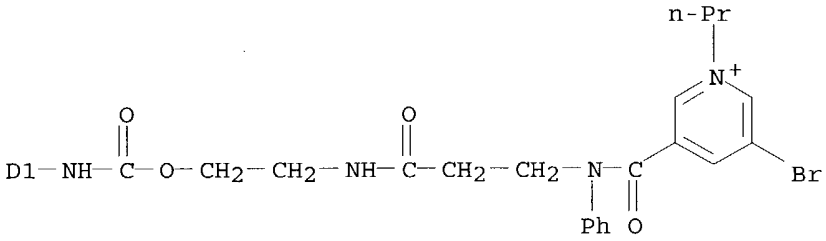
IT **121447-89-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as platelet activating factor antagonist)

RN 121447-89-0 HCAPLUS

CN Pyridinium, 3-bromo-5-[[[3-[[2-[[[(butylphenyl)amino]carbonyl]oxy]ethyl]amino]-3-oxopropyl]phenylamino]carbonyl]-1-propyl-, chloride (9CI) (CA INDEX NAME)

PAGE 1-A

D1— Bu-n



PAGE 2-A

● Cl^-

L42 ANSWER 70 OF 101 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1987:636355 HCAPLUS
DN 107:236355
ED Entered STN: 25 Dec 1987
TI 1-Methylcarbapenems having an externally alkylated mono- or bicyclic 2-quaternary heteroarylalkylthio substituent
IN Christensen, Burton G.; Johnston, David B. R.; Schmitt, Susan M.
PA Merck and Co., Inc., USA
SO Eur. Pat. Appl., 174 pp.
CODEN: EPXXDW
DT **Patent**
LA English
IC ICM C07D487-04
ICS A61K031-40; C07D519-00
CC 26-5 (Biomolecules and Their Synthetic Analogs)
Section cross-reference(s): 1
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI EP 170073	A1	19860205	EP 1985-108132	19850701 <--
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
CA 1273012	A1	19900821	CA 1985-485383	19850626 <--
DK 8502975	A	19860314	DK 1985-2975	19850701 <--
ES 544751	A1	19860901	ES 1985-544751	19850701 <--
JP 61083183	A2	19860426	JP 1985-145659	19850702 <--
PRAI US 1984-626821		19840702 <--		

GI For diagram(s), see printed CA Issue.
AB Carbapenems I [L = covalent bond, (CH2)1-4S, (CH2)1-4O, (CH2)1-4X(CH2)1-4; X = O, S, N(C1-6 alkyl), which may be (un)substituted; Q is a substituted mono- or bicyclic heteroarylium group], useful as antibiotics (no data),

were prepared by 4 methods. Phosphate II [R = OP(O)(OPh)2] in MeCN was treated with EtN(CHMe2)2 and 2-pyridylmethylmercaptan 3 h at 0° to give II (R = 2-pyridylmethylthio) which was quaternized with FSO3Me to give II (R = 1-methyl-2-pyridiniumylmethylthio fluorosulfonate). Hydrogenolysis gave the inner salt III.

ST antibiotic quaternary carbapenem prepn; penem quaternary carba antibiotic prepn

IT Antibiotics
(quaternary carbapenem derivs.)

IT 78852-98-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(dehydropeptidase inhibitor, combination of, with quaternary carbapenem derivs.)

IT 6086-21-1, 1-Methyl-1,2,4-triazole
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydroxymethylation of)

IT 104256-50-0P 104256-54-4P 104256-64-6P 104256-66-8P 104278-62-8P
104278-64-0P 104298-73-9P 105617-70-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrogenolysis of)

IT 104256-51-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)

IT 59020-97-2P 91616-37-4P 104256-47-5P 104256-56-6P 104256-63-5P
104256-67-9P 104278-61-7P 105557-92-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and quaternization of)

IT 104256-61-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of)

IT 104256-71-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with carbapenemyl phosphate derivative)

IT 16927-00-7P 104256-69-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with potassium thioacetate)

IT 91616-36-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with thionyl chloride)

IT 91616-39-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with trifluoromethanesulfonic acid)

IT 104256-86-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT 91616-40-9P 104256-48-6P 104256-52-2P 104256-55-5P 104256-58-8P
104256-59-9P 104256-62-4P 104256-65-7P 104256-68-0P 104256-73-7P
104256-74-8P 104256-75-9P 104256-76-0P 104256-77-1P 104256-78-2P
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RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of, as antibiotic)

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RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of, as antibiotic)

IT 421-20-5, Methyl fluorosulfonate
RL: RCT (Reactant); RACT (Reactant or reagent)
(quaternization by, of nitrogen heterocyclyl alkylthiolcarbapenems)

IT 35250-75-0, 2-Picolyl thioacetate
RL: RCT (Reactant); RACT (Reactant or reagent)
(quaternization of)

IT 2044-73-7 16133-26-9 17617-05-9 27349-73-1 53062-92-3 70199-58-5 104256-53-3 104256-57-7, 4-Thiazolemethanethiol
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with carbapenemyl phosphate derivative)

IT 90776-59-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with mercaptans)

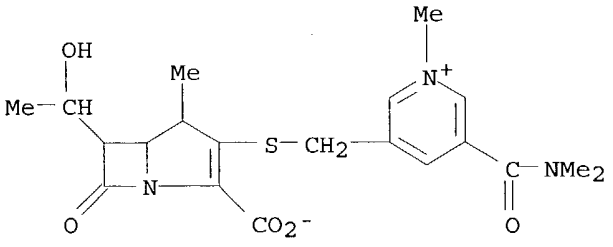
IT 10387-40-3, Potassium thioacetate
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with pyridylethyl chloride)

IT 103-74-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with thionyl chloride)

IT **104280-33-3P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of, as antibiotic)

RN 104280-33-3 HCAPLUS
CN Pyridinium, 3-[[[2-carboxy-6-(1-hydroxyethyl)-4-methyl-7-oxo-1-

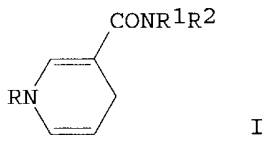
azabicyclo[3.2.0]hept-2-en-3-yl]thio]methyl]-5-[(dimethylamino)carbonyl]-1-methyl-, inner salt (9CI) (CA INDEX NAME)



L42 ANSWER 75 OF 101 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1986:119924 HCAPLUS
DN 104:119924
ED Entered STN: 05 Apr 1986
TI Electrophotographic photosensitive materials
IN Kobayashi, Toyoko; Miyazaki, Hajime
PA Canon K. K., Japan
SO Jpn. Kokai Tokkyo Koho, 18 pp.
CODEN: JKXXAF
DT **Patent**
LA Japanese
IC ICM G03G005-06
ICS C07D211-90; H01L031-08
CC 74-3 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI JP 60184252	A2	19850919	JP 1984-38708	19840302 <--
PRAI JP 1984-38708		19840302 <--		

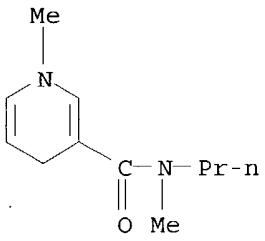
GI



I

AB Electrophotog. photosensitive materials contain a dihydronicotinamide I (R = H, alkyl, aralkyl; R1, R2 = H, amino, alkyl, aralkyl, alkenyl, aryl). I is especially useful as a charge carrier-transporting agent in composite electrophotog. photoreceptors. Thus, an Al support was coated with a composition containing β-type Cu phthalocyanine and a polyester binder and coated with a composition containing I (R = R1 = R2 = H) and a polycarbonate resin to give an electrophotog. photoreceptor having high sensitivity, small dark decay, and excellent durability.
ST electrophotog charge transport agent dihydronicotinamide; nicotinamide dihydro charge transfer agent
IT Photography, electro-, photoconductors
(composite, charge carrier-transporting agents for, nicotinamide

derivs., as)
IT 17750-24-2 18940-08-4 63942-72-3 76377-78-1 100780-95-8
100780-96-9 **100780-97-0** 100780-98-1 100780-99-2
100781-00-8 100781-01-9 100781-02-0 **100781-03-1**
100781-04-2 100781-05-3 **100781-06-4** 100781-07-5
100781-08-6
RL: USES (Uses)
(electrophotog. charge carrier-transporting agent)
IT 5096-13-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrogenation of)
IT 952-92-1P
RL: PREP (Preparation)
(preparation of, as electrophoto. charge carrier-transporting agent)
IT 98-92-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with benzyl chloride)
IT 100-44-7, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with nicotinamide)
IT **100780-96-9**
RL: USES (Uses)
(electrophotog. charge carrier-transporting agent)
RN 100780-96-9 HCAPLUS
CN 3-Pyridinecarboxamide, 1,4-dihydro-N,1-dimethyl-N-propyl- (9CI) (CA INDEX NAME)



L42 ANSWER 80 OF 101 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1982:472194 HCAPLUS
DN 97:72194
ED Entered STN: 12 May 1984
TI Imidazorifamycins, their pharmaceutical preparations and their use
IN Kump, Wilhelm; Traxler, Peter; Scartazzini, Riccardo
PA Ciba-Geigy A.-G. , Switz.
SO Eur. Pat. Appl., 97 pp.
CODEN: EPXXDW
DT **Patent**
LA German
IC C07D498-18; C07D498-08; A61K031-335
ICI C07D498-18, C07D307-00, C07D267-00, C07D235-00; C07D498-08, C07D307-00, C07D267-00
CC 26-6 (Biomolecules and Their Synthetic Analogs)
Section cross-reference(s): 1
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

PI	EP 49683	A2	19820414	EP 1981-810387	19810921 <--
	EP 49683	A3	19820901		
	R: AT, BE, CH, DE, FR, IT, LU, NL, SE				
	FI 8102936	A	19820326	FI 1981-2936	19810921 <--
	DD 204925	A5	19831214	DD 1981-247258	19810921 <--
	AU 8175594	A1	19820401	AU 1981-75594	19810923 <--
	GB 2084575	A	19820415	GB 1981-28704	19810923 <--
	ES 505723	A1	19821201	ES 1981-505723	19810923 <--
	NO 8103258	A	19820326	NO 1981-3258	19810924 <--
	DK 8104219	A	19820326	DK 1981-4219	19810924 <--
	ZA 8106635	A	19820929	ZA 1981-6635	19810924 <--
	JP 57085393	A2	19820528	JP 1981-151931	19810925 <--
	ES 514883	A1	19830601	ES 1982-514883	19820810 <--
PRAI	CH 1980-7184		19800925 <--		
	CH 1980-7185		19800925 <--		

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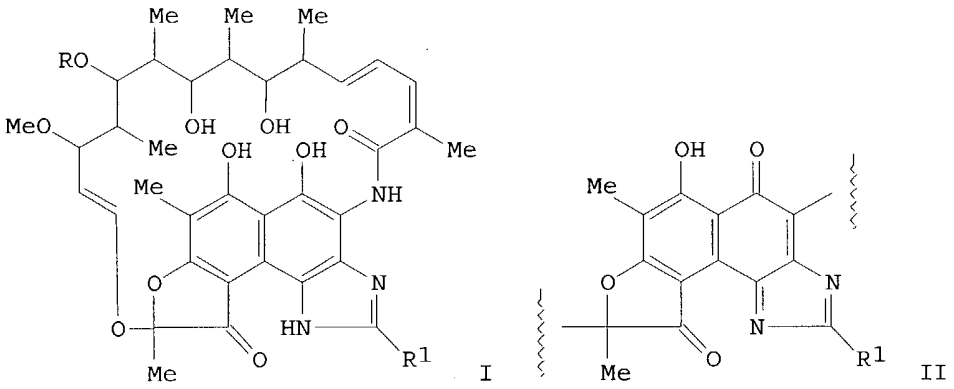

AB Rifamycins SV (I) and S (II, R = H, Ac; R1 = secondary amino) were prepared Thus 3-amino-4-iminorifamycin S was treated with Me2NCH(OMe)2 to give I (R = Ac, R1 = NMe2) which had a min. inhibitory concentration of 0.005 μg/mL against Staphylococcus aureus 2999.

ST aminoimidazorifamycin prepn bactericide; rifamycin aminoimidazo prepn bactericide; imidazorifamycin prepn bactericide

IT Bactericides, Disinfectants, and Antiseptics
(aminoimidazorifamycins)

IT 617-84-5 4394-85-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(chlorination of)

IT 79540-42-4P 79540-43-5P 79540-44-6P 79540-45-7P 79540-48-0P
79553-71-2P 82499-86-3P 82499-88-5P 82499-90-9P 82499-93-2P
82499-95-4P 82499-98-7P 82500-00-3P 82500-03-6P 82500-05-8P
82500-07-0P 82500-09-2P 82500-11-6P 82500-13-8P 82500-15-0P
82500-17-2P 82500-19-4P 82500-21-8P 82500-24-1P 82500-26-3P
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82516-48-1P 82534-52-9P 82534-53-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and bactericidal activity of)

IT 5211-86-9P 5211-95-0P 5564-73-8P 22630-09-7P 28568-56-1P
32895-16-2P 54172-24-6P 54172-25-7P 82499-85-2P 82499-87-4P
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RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with aminoiminorifamycin)

IT 82502-21-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with aminoiminorifamycin S)

IT 69479-71-6P 82516-38-9P 82516-40-3P 82516-49-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with aminorifamycin)

IT 4429-01-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with aminorifamycin S)

IT 80026-30-8P 82516-34-5P 82516-44-7P 82516-50-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with ammonia)

IT 79540-44-6P 82502-23-6P 82502-79-2P 82516-33-4P 82516-51-6P
82516-53-8P 82516-56-1P 82516-59-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT 82502-26-9P 82516-35-6P 82516-36-7P 82516-37-8P 82516-39-0P
82516-41-4P 82516-42-5P 82516-43-6P 82516-45-8P 82516-46-9P
82516-47-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, reaction with ammonia, and bactericidal activity of)

IT 82516-32-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, reduction, and bactericidal activity of)

IT 92-54-6 103-67-3 105-04-4 109-01-3 110-68-9 110-73-6 110-89-4, reactions 110-91-8, reactions 111-49-9 111-95-5 120-43-4
122-07-6 123-75-1, reactions 123-90-0 141-91-3 142-25-6 142-84-7
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82516-03-8 82516-06-1 82516-17-4 82516-24-3 82516-29-8
82516-54-9 82516-57-2 82534-54-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with DMF di-Me acetal)

IT 4637-24-5 5762-56-1 19449-31-1 82502-24-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with aminoiminorifamycin)

IT 7664-41-7, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with aminomethyleneaminorifamycins)

IT 82502-22-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with aminorifamycin S)

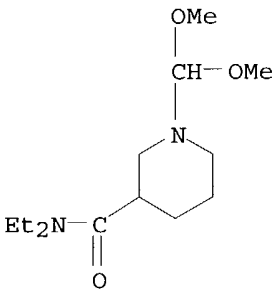
IT 6282-00-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with di-Me sulfate)

IT 62041-01-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with formamide di-Me acetals)

IT 51756-80-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with formylpiperazine di-Me acetal)

IT **82502-59-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with aminoiminorifamycin)

RN 82502-59-8 HCAPLUS
CN 3-Piperidinecarboxamide, 1-(dimethoxymethyl)-N,N-diethyl- (9CI) (CA INDEX NAME)

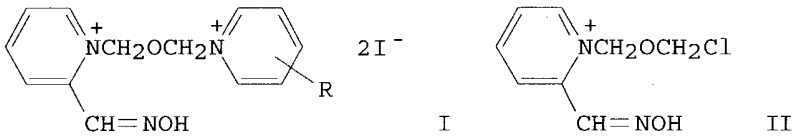


L42 ANSWER 85 OF 101 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1978:50664 HCAPLUS
DN 88:50664
ED Entered STN: 12 May 1984
TI Bis(quaternary pyridinium)-2-aldoxime salts
IN Hagedorn, Ilse
PA Merck Patent G.m.b.H., Fed. Rep. Ger.

SO Ger. Offen., 19 pp.
CODEN: GWXXBX
DT **Patent**
LA German
IC C07D401-12
CC 27-17 (Heterocyclic Compounds (One Hetero Atom))
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 2616481	A1	19771103	DE 1976-2616481	19760414 <--
	FR 2348211	A1	19771110	FR 1977-10729	19770408 <--
	FR 2348211	B1	19800418		
	US 4128651	A	19781205	US 1977-786693	19770411 <--
	IL 51857	A1	19800530	IL 1977-51857	19770411 <--
	DK 7701631	A	19771015	DK 1977-1631	19770413 <--
	SE 7704240	A	19771015	SE 1977-4240	19770413 <--
	NL 7704030	A	19771018	NL 1977-4030	19770413 <--
	ZA 7702253	A	19780329	ZA 1977-2253	19770413 <--
	GB 1516626	A	19780705	GB 1977-15341	19770413 <--
	CA 1070307	A1	19800122	CA 1977-276042	19770413 <--
	AT 7702570	A	19800915	AT 1977-2570	19770413 <--
	AT 361923	B	19810410		
	CH 627745	A	19820129	CH 1977-4592	19770413 <--
	BE 853570	A1	19771014	BE 1977-55827	19770414 <--
	JP 52128381	A2	19771027	JP 1977-43425	19770414 <--
	ES 457791	A1	19780801	ES 1977-457791	19770414 <--
PRAI	DE 1976-2616481		19760414 <--		

GI



AB Iodides I (R = 3-, 4-acyl, carbamoyl, alkoxycarbonyl) (37 compds.) were prepared for the treatment of poisoning by organophosphorus pesticides or warfare agents, e.g. Soman (no data). Treatment of the iodides with AgCl or AgBr gave the chlorides or bromides, resp. I (R = 3-Bz) was prepared by treating II with 3-benzoylpyridine and NaI.
ST pyridiniummethyl ether salt; poisoning organophosphorus antidote
IT Poisoning
(organophosphorus, bis(pyridiniummethyl) ether salts in treatment of)
IT Pesticides
(organophosphorus, poisoning by, bis(pyridiniummethyl) ether salts in treatment of)
IT Chemical warfare agents
(poisoning by, bis(pyridiniummethyl) ether salts in treatment of)
IT 96-64-0 7723-14-0D, organic derivs.
RL: RCT (Reactant); RACT (Reactant or reagent)
(bis(pyridiniummethyl) ether salts in treatment of poisoning by)
IT 65320-89-0P 65320-90-3P 65320-91-4P 65320-92-5P 65320-93-6P
65320-94-7P 65320-95-8P 65320-96-9P 65320-97-0P 65320-98-1P
65320-99-2P 65321-00-8P 65321-01-9P 65321-02-0P 65321-03-1P
65321-04-2P 65321-05-3P 65321-06-4P 65321-07-5P 65321-08-6P
65321-09-7P 65321-10-0P 65321-11-1P **65321-12-2P**
65321-13-3P 65321-14-4P 65321-15-5P 65321-16-6P

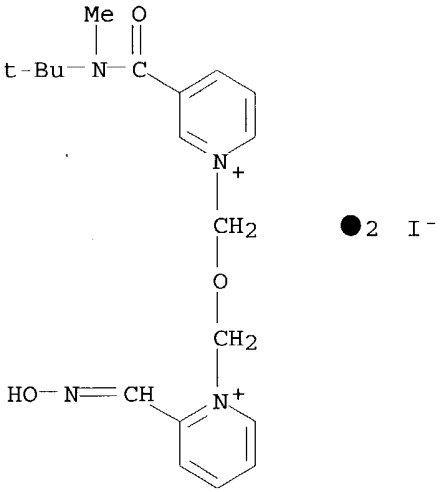
65321-17-7P 65321-18-8P 65321-19-9P 65321-20-2P 65321-21-3P
65321-22-4P 65321-23-5P 65321-24-6P 65321-25-7P 65321-26-8P
65321-27-9P 65321-28-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT 94-44-0 350-03-8 553-60-6 614-18-6 1017-24-9 1752-96-1
2503-55-1 3034-31-9 3468-53-9 4314-66-3 5424-19-1 6938-06-3
7681-15-4 10254-15-6 10354-56-0 14548-46-0 14627-92-0 15828-08-7
23826-71-3 24303-05-7 34950-04-4 60148-00-7 61780-09-4
65035-97-4 65321-29-1 65321-30-4 65321-31-5 65321-32-6
65321-33-7 65321-34-8 65321-35-9 65321-36-0 65321-37-1
65321-38-2 65321-39-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with chloromethoxymethylpyridine chloride derivative)

IT 27123-11-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with pyridine)

IT **65321-12-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 65321-12-2 HCAPLUS
CN Pyridinium, 1-[[[3-[[(1,1-dimethylethyl)methylamino]carbonyl]pyridinio]methoxy]methyl]-2-[(hydroxyimino)methyl]-, diiodide (9CI) (CA INDEX NAME)



L42 ANSWER 90 OF 101 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1974:82697 HCAPLUS
DN 80:82697
ED Entered STN: 12 May 1984
TI 1,4-Dihydropyridinecarboxamides
IN Bossert, Friedrich; Meyeer, Horst; Vater, Wulf; Stoepel, Kurt
PA Bayer A.-G.
SO Ger. Offen., 44 pp.
CODEN: GWXXBX
DT **Patent**
LA German
IC C07D
CC 27-17 (Heterocyclic Compounds (One Hetero Atom))
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 2228377	A1	19740103	DE 1972-2228377	19720610 <--
	BE 800680	A1	19731210	BE 1973-132065	19730608 <--
	FR 2187349	A1	19740118	FR 1973-21038	19730608 <--
PRAI	DE 1972-2228377		19720610 <--		

GI For diagram(s), see printed CA Issue.

AB Eighteen amides I (R = H or Me; R1 = NH2, NHMe, NHCHMe2, NHCMe3, NMe2, or morpholino; R2 = e.g. 2-, 3-, or 4-pyridyl, 3-NCC6H4, 3-O2NC6H4, or 3-F3CC6H4; R3 = e.g. CONH2, CONHMe, or CO2Et) of low toxicity and useful as antihypertensives and in the treatment of cardiac disorders were manufactured Thus, refluxing 2-pyridine-carboxaldehyde, MeCOCH2CONH2 (II), and concentrated NH4OH in EtOH gave 56% I (R = H, R1 = NH2, R2 = 2-pyridyl, R3 = CONH2). Refluxing 3-O2NC6H4CH:CHCOCH2CO2Et, II and concentrated NH4OH in EtOH gave 58% I (R = H, R1 = NH2, R2 = 3-O2NC6H4, R3 = CO2Et).

ST pyridinecarboxamide antihypertensive; heart treatment pyridinecarboxamide

IT Condensation reaction
(cyclo-, of pyridinecarboxaldehyde with amide and ammonia)

IT Antihypertensives
(dihydropyridinecarboxamides)

IT Heart, disease or disorder
(dihydropyridinecarboxamides in treatment of)

IT 5977-14-0 20306-75-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with ammonia and carboxaldehydes)

IT 89-98-5 99-61-6 447-61-0 454-89-7 500-22-1 552-89-6 872-85-5 1121-60-4 15725-23-2 24964-64-5 39562-16-8 39562-33-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation reaction with amides and ammonia)

IT 593-51-1 7664-41-7, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation with amides and carboxaldehydes)

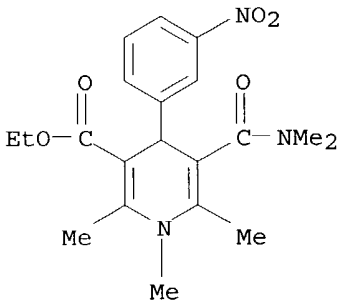
IT 2044-64-6 24486-56-4 41153-91-7 42222-06-0 51423-43-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation with ammonia and carboxaldehydes)

IT 51423-25-7P 51423-26-8P 51423-27-9P 51423-28-0P 51423-29-1P 51423-30-4P 51423-31-5P 51423-32-6P 51423-33-7P 51423-34-8P 51423-35-9P 51423-36-0P 51423-37-1P 51423-38-2P 51423-39-3P 51423-40-6P **51423-41-7P** 51423-42-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT **51423-41-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 51423-41-7 HCAPLUS

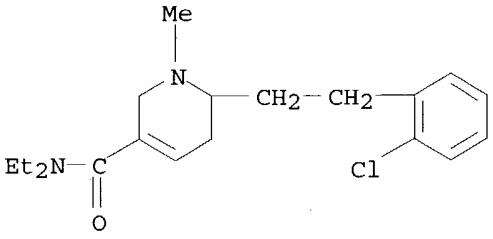
CN 3-Pyridinecarboxylic acid, 5-[(dimethylamino)carbonyl]-1,4-dihydro-1,2,6-trimethyl-4-(3-nitrophenyl)-, ethyl ester (9CI) (CA INDEX NAME)



L42 ANSWER 95 OF 101 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1970:100543 HCAPLUS
DN 72:100543
ED Entered STN: 12 May 1984
TI N,N-Diethyl-4-methyl-2,3,4,4a,5,6-hexahydrobenzo[f]quinoline-2-carboxamide
IN Julia, Marc; Igolen, Jean
PA Institut Pasteur
SO Fr., 2 pp.
CODEN: FRXXAK
DT **Patent**
LA French
IC C07C
CC 27 (Heterocyclic Compounds (One Hetero Atom))
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	FR 1555553		19690131	FR	19670705 <--
	DE 1770809			DE	
	GB 1238940			GB	

GI For diagram(s), see printed CA Issue.
AB The title compound (I) was prepared by the KBH4 reduction of N,N-diethyl-1-methyl-6-(o-chlorophenethyl)nicotinamide (II), and the resulting 1,2,5,6-tetrahydro derivative treated with KNH2 in liquid NH3 at -33 to +15°. Thus, 1.7 g KBH4 was added in portions over 10 min to a stirred solution of 7.2 g II in 150 ml MeOH and 150 ml H2O and stirring continued 2 hr to give 3.2 g N,N-diethyl-1-methyl-6-(o-chlorophenethyl)-1,2,5,6-tetra-hydronicotinamide (III), b0.01 164-6°; oxalate m. 83-6° (alc. Et2O). K (13.8 g) was added over 15 min to 1500 ml liquid NH3 in the presence of Fe(NO3)3, after 0.5 hr a solution of 29.5 g III in 50 ml anhydrous Et2O added rapidly, the mixture stirred 45 min, excess NH4Cl added, NH3 evaporated with a stream of air, and the residue worked up to give 16 g I; oxalate m. 168-70° (EtOH).
ST benzoquinolines hexahydro; quinolines hexahydrobenzo
IT **21173-34-2P** 26181-46-4P **26920-78-5P** 26920-79-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT **21173-34-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 21173-34-2 HCAPLUS
CN Nicotinamide, 6-(o-chlorophenethyl)-N,N-diethyl-1,2,5,6-tetrahydro-1-methyl- (8CI) (CA INDEX NAME)



L42 ANSWER 101 OF 101 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1963:403566 HCAPLUS
DN 59:3566
OREF 59:639a-c
ED Entered STN: 22 Apr 2001
TI 3-(4-Azaphenothiazino)propylnipecotic and -isonipecotic acids
PA Deutsche Gold- und Silber-Scheideanstalt vorm. Roessler
SO 16 pp.
DT **Patent**
LA Unavailable
CC 38 (Heterocyclic Compounds (More Than One Hetero Atom))

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
PI	BE 620056		19621031	BE		<--
	DE 1159464			DE		
	GB 993748			GB		
PRAI	DE		19610712	<--		

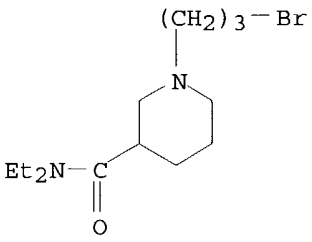
GI For diagram(s), see printed CA Issue.
AB Amides and esters of the title acids can be used to lower blood pressure. N,N-Diethylnicotinamide 178, NaBr 103, and Cl(CH2)3OH 95 is heated at 140° for 1 hr., the NaCl that forms is filtered off, and the filtrate hydrogenated in MeOH under 5 atmospheric at room temperature in the presence of 1 g. PtO2 to give N,N-diethyl-1-(3-hydroxypropyl)nipecotinamide (I) 132 parts. I 25 and 66% HBr 120 is refluxed for 3 hrs. to give N,N-diethyl-1-(3-bromopropyl)nipecotinamide (II) 31 parts. 4-Azaphenothiazine 20 and PhMe 150 are refluxed, 50% NaNH2 in PhMe 8 is added in portions, the mixture refluxed for 30 min., II 31 dissolved in PhMe 100 added in 20 min., the mixture refluxed 2 hrs., cooled, and treated with H2O. The reaction mixture is washed twice with H2O, extracted with HCl, the HCl solution extracted with NaOH and C6H6, and the C6H6 evaporated to give N,N-diethyl-1-[3-(4-aza- phenothiazino)propyl]nipecotinamide-HCl iso-PrOH solvate, m. 134-5°. Similarly prepared are III (R, R1, position of CONRR1 group and m.p. given): H, H, 4, 214-17°; Me, Me, 4,212-13° (iso-PrOH); Et, Et, 4, 140-1°; Me, H, 4, 195-6°; (NRR1 =) piperidino, 4, 174-5°.
IT Isonipecotic acid, 1-[3-(10H-pyrido[3,2-b][1,4]benzothiazin-10-yl)propyl]-
Nipecotic acid, 1-[3-(10H-pyrido[3,2-b][1,4benzothiazin-10-yl)propyl]-
(derivs.)
IT 261-96-1, 10H-Pyrido[3,2-b][1,4]benzothiazine
(derivs.)
IT **92156-24-6**, Nipecotamide, 1-(3-bromopropyl)-N,N-diethyl-
92168-64-4, Nipecotamide, N,N-diethyl-1-(3-hydroxypropyl)-
99870-51-6, Isonipecotamide, 1-[3-(10H-pyrido[3,2-b][1,4]benzothiazin-10-yl)propyl]-, hydrochloride 100457-55-4, Phenothiazine, 2-chloro-10-[3-(hexahydro-1H-azepin-1-yl)propyl]-, hydrochloride
100626-64-0, Isonipecotamide, N-methyl-1-[3-(10H-pyrido[3,2-b][1,4]-

benzothiazin-10-yl)propyl]-, hydrochloride 100931-04-2, Phenothiazine, 10-[3-(hexahydro-1H-azepin-1-yl)propyl]-, hydrochloride 101176-21-0, Isonipecotamide, N,N-diethyl-1-[3-(10H-pyrido[3,2-b][1,4]-benzothiazin-10-yl)propyl]-, hydrochloride **101176-22-1**, Nipecotamide, N,N-diethyl-1-[3-(10H-pyrido[3,2-b][1,4]benzothiazin-10-yl)propyl]-, hydrochloride 101612-59-3, Isonipecotamide, N,N-dimethyl-1-[3-(10H-pyrido[3,2-b][1,4]benzothiazin-10-yl)propyl]-, hydrochloride 104780-96-3, Isonipecotic acid, 1-[3-(10H-pyrido[3,2-b][1,4]benzothiazin-10-yl)propyl]-, ethyl ester 106684-04-2, Piperidine, 1-[1-[3-(10H-pyrido[3,2-b][1,4]benzothiazin-10-yl)propyl]isonipecotoyl]-, hydrochloride
(preparation of)

IT **92156-24-6**, Nipecotamide, 1-(3-bromopropyl)-N,N-diethyl-
(preparation of)

RN 92156-24-6 HCAPLUS

CN Nipecotamide, 1-(3-bromopropyl)-N,N-diethyl- (7CI) (CA INDEX NAME)



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STRUCTURE FILE UPDATES:   13 JUL 2004  HIGHEST RN 709042-93-3
DICTIONARY FILE UPDATES:  13 JUL 2004  HIGHEST RN 709042-93-3

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

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Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
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http://www.cas.org/ONLINE/DBSS/registryss.html

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L9             1 SEA FILE=REGISTRY ABB=ON  PLU=ON  "CB 1954"/CN


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YOU HAVE REQUESTED DATA FROM FILE 'HCAPLUS' - CONTINUE? (Y)/N:n


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OTHER NAMES:
CN   2,4-Dinitro-5-ethyleneiminobenzamide
CN   2,4-Dinitroethyleneiminobenzamide
CN   5-(1-Aziridinyl)-2,4-dinitrobenzamide
CN   5-Aziridino-2,4-dinitrobenzamide
CN   5-Aziridinyl-2,4-dinitrobenzamide
CN   CB 1954
CN   NSC 115829
MF   C9 H8 N4 O5
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       BIOTECHNO, CA, CANCERLIT, CAPLUS, CASREACT, CHEMCATS, CIN, DDFU, DRUGU,
       EMBASE, IMSDRUGNEWS, IMSRESEARCH, MEDLINE, PROMT, PROUSDDR, RTECS*,
       TOXCENTER, USPAT2, USPATFULL
         (*File contains numerically searchable property data)
DT.CA  CAplus document type:  Conference; Dissertation; Journal; Patent
RL.P   Roles from patents:  ANST (Analytical study); BIOL (Biological study);
       PROC (Process); RACT (Reactant or reagent); USES (Uses)
RLD.P  Roles for non-specific derivatives from patents:  BIOL (Biological
       study); USES (Uses)
RL.NP  Roles from non-patents:  ANST (Analytical study); BIOL (Biological
       study); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP
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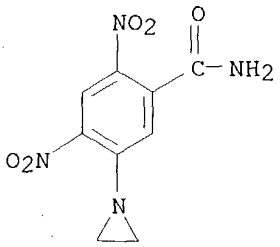
(Properties); RACT (Reactant or reagent); USES (Uses)
RLD.NP Roles for non-specific derivatives from non-patents: BIOL (Biological study); PRP (Properties)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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4 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
153 REFERENCES IN FILE CAPLUS (1907 TO DATE)

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L12 0 SEA FILE=REGISTRY ABB=ON PLU=ON L10 AND L11

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